AD NUMBER

AD851126

NEW LIMITATION CHANGE

TO

Approved for public release, distribution unlimited

FROM

Distribution authorized to U.S. Gov't. agencies and their contractors; Administrative/Operational Use; DEC 1969. Other requests shall be referred to Edgewood Arsenal, Attn: SMUEA-TSTI-T, Edgewood Arsenal, MD 21010.

AUTHORITY

US Army Edgewood Arsenal notice dtd 21 Apr 1970

AD

CIDS No. 6

HANDBOOK OF CIDS
CHEMICAL SEARCH COMPONENTS

Status Report

by

Clarence T. Van Meter

Eric N. Goldschmidt

Margaret Milne

December 1968

DEPARTMENT OF THE ARMY
EDGEWOOD ARSENAL
Technical Support Directorate
Technical Data Coordination Office
Edgewood Arsenal, Maryland 21010

Contract DA-18-035-AMC-288(A)

UNIVERSITY OF PENNSYLVANIA
PHILADELPHIA PENNSYLVANIA 19104

205

CIDS No. 6

HANDBOOK OF CIDS CHEMICAL SEARCH COMPONENTS

Status Report

by

Clarence T. Van Meter
Eric N. Goldschmidt
Margaret Milne

December 1968

DEPARTMENT OF THE ARMY
EDGEWOOD ARSENAL

Technical Support Directorate
Technical Data Coordination Office
Edgewood Arsenal, Maryland 21010

Contract DA-18-035-AMC-288(A)

Task 2P062101A72702

UNIVERSITY OF PENNSYLVANIA

Philadelphia, Pennsylvania 19104

FOREWORD

The work described in this report was authorized under Task 2P062101A72702, Army Chemical Information and Data Systems (U). The work was started in July 1964 and is continuing. The information contained in this report represents part of the work accomplished primarily during the calendar year 1968.

The report is pre-punched with holes to permit insertion in a standard three-ring binder, after removal of the staples, thus facilitating use as a desk top tool.

The information in this document has not been cleared for release to the general public.

Acknowledgment

The authors are pleased to acknowledge the continuous assistance of Mrs. Ruth V. Powers in all matters germane to compatibility of chemical representation with CIDS computer programming. Grateful appreciation is also expressed for the generous cooperation of members of the staff of the Technical Data Coordination Office and the EDP Systems personnel, Edgewood Arsenal.

The authors are also grateful for the generous assistance of Miss Mary Jane Potter in performing all of the art work, and of Col. Frank M. Steadman in providing editorial guidance.

DIGEST

This handbook presents a display of the chemical search components of CIDS which are designed for use via computer to effect rapid discrimination among chemical compounds currently admitted to the system. The computer programming necessary to incorporate these components into the working system is in process and the expectation is that this incorporation will be effected during the early months of the model operational CIDS.

The search components subdivide into two general types depending on whether they describe characteristics discernible through probes of molecular formulas or of structural formulas. The latter type is by far the more numerous and consists of several hundred substructural features (structural fragments) which function as search keys (screens) in the automated system.

The handbook is intended to serve as a desk-top tool in the intellectual assignment of CIDS chemical search keys to queries addressed to the system. The information is presented from the point of view of the chemist, i.e., it permits stipulation, in conventional chemical fashion, of all features of chemistry appropriate to a query but does not prescribe for the transformation of this information into a formal computer query. The latter will be provided in another CIDS publication.

In the interest of practical utility, a very deliberate effort has been made to subdivide the structural fragment keys into conventional categories which will therefore appeal to the practicing chemist. A description of each category is provided and, wherever appropriate, the individual keys within each category are shown (a) in molecular formula style, (b) structured, and (c) associated with their CIDS code designations. Generous use is made of the tabular method of presenting the keys and the ordering of the keys in each table is especially designed to facilitate rapid location of any individual key. Nomenclature indexes are provided for the three large categories of structural fragment keys, viz., specific cyclic nuclei, specific functional groups, and hydrocarbon radicals.

The concluding section of the report provides illustrations of the assignment of the chemical search keys to a wide structural spectrum of compounds.

It is emphasized that each illustration portrays all of the chemical search keys which will be assigned to a compound automatically (by computer) at the time the compound is registered into the CIDS file. Only a small family of these keys will be appropriate to a particular query, and the composition of this small family will vary according to the nature of the query.

TABLE OF CONTENTS

LIST OF TABLES

HANDBOOK OF CIDS CHEMICAL SEARCH COMPONENTS

1. INTRODUCTION

The primary purpose of this publication is to provide a categorized disclosure of all features of molecular composition and structure which have been incorporated into the initial model of an operational Chemical Information and Data System (CIDS). The categorization and the ordering of the features within each category are deliberately designed to facilitate employment of the publication as a desk top tool during operations associated with the selection of chemical search keys in the formulation of computer queries.

The presentation in this publication supersedes that contained in Section 3 of the CIDS No. 4 publication (1). The earlier presentation was designed for use in an experimental system whereas this presentation constitutes a revision which incorporates the findings of that experimentation. The experimental work continued over a period of about 18 months and involved the formulation and processing of several hundred queries, a sizable proportion of which originated from extra-Project sources.

The development of this initial model of an operational system represents another stage in the orderly evolution of a fully operational system. Indeed, the primary purpose of the model system is to demonstrate the feasibility of proceeding to a fully operational system having acceptable features of practical utility. It is thus understandable that no attempt is made in this publication to provide search keys adequate for all structural types of chemical compounds. It is estimated that the keys which are provided will suffice for upwards of 90 percent of the organic compounds contained in the sponsor's files submitted for the study. Certain types of compounds, e.g., inorganics, polymers, coordination complexes, glycosides, etc., are not yet admitted to the system. Acceptable techniques have been formulated for handling the chemistry of many of these presently unadmitted classes, and the necessary computer programming will be undertaken as future time permits. Concomitant with programming accomplishments, the presentation in this handbook will be updated.

2. THE SEARCH COMPONENTS

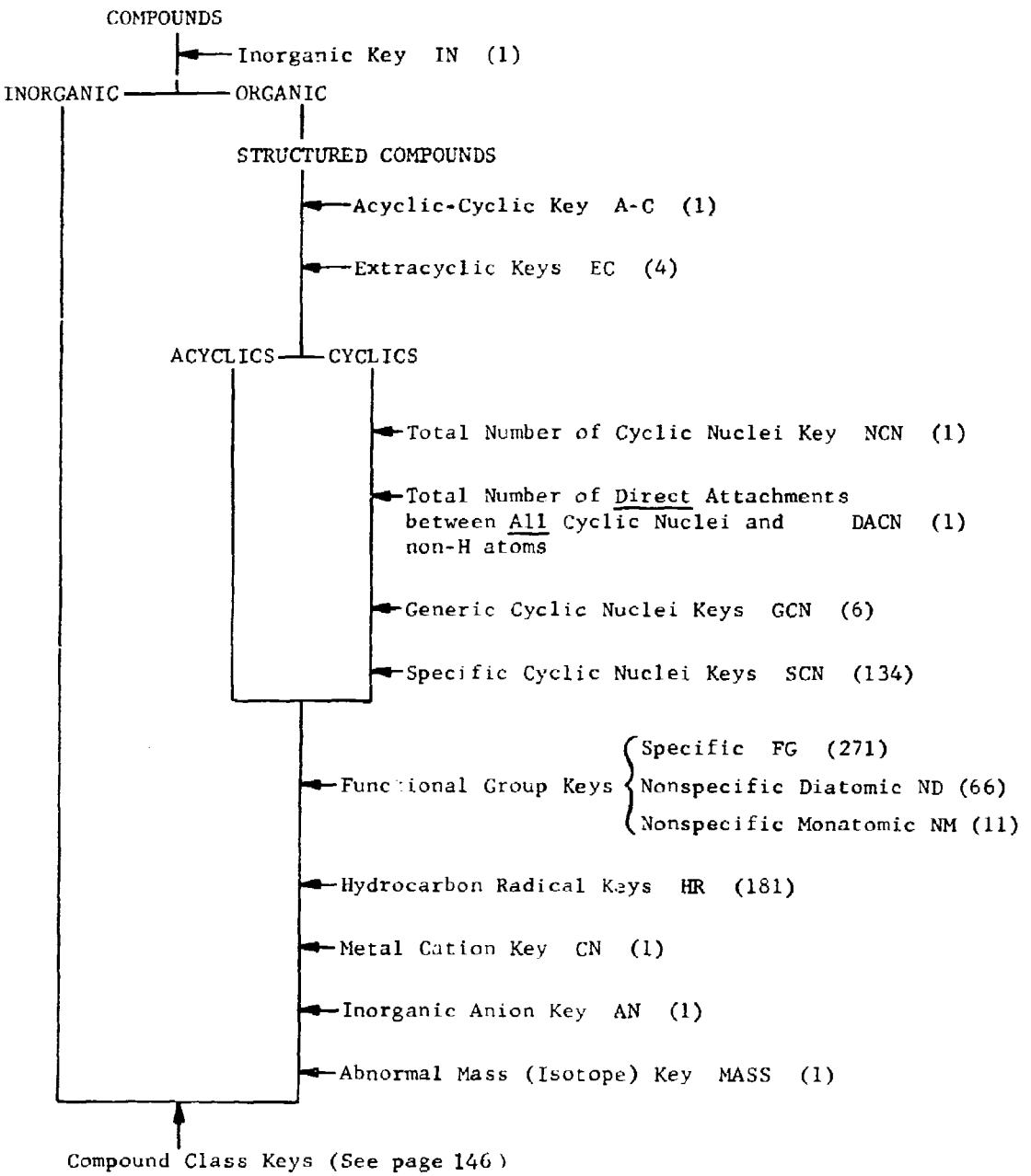
For rapid machine discrimination among chemical compounds, CIDS employs two kinds of search components, viz., (1) Molecular Formula Keys & Statements, and (2) Structural Fragment Keys. As the names imply, the former utilizes only that information conveyed by the molecular formula, whereas the latter embodies all substructural features portrayed in the structural formula.

Judicious employment of these search components renders feasible the rapid processing of structural queries addressed to the system. Depending on the nature of the query, the retrieved compounds may all be true respondents or they may be a mixture of true respondents and compounds of closely related structure. In the latter case, the true respondents may be identified either by visual examination of the printed out structures or by an atom-by-atom computer search.

Although searches based exclusively on molecular formula information are feasible, operation of the system is not predicated on an initial discrimination in terms of molecular formulas. In the interest of economy of search, it is often desirable to probe first on the basis of substructural features and then impose, if necessary, molecular formula restrictions. The reader will recognize this as opposite to the scheme employed in various works of reference utilizing molecular formula indexes. A similar CIDS molecular formula index will be available as a desk top tool.

An overview of the several kinds of structural search keys embodied in the system is provided in Table I. It will be observed that the single IN key serves to subdivide the total file into inorganic and organic compounds. Discriminative keys for the inorganic compounds are not shown since, although formulated, they remain to be incorporated into the working system. The organic structure keys are subdivided on the basis of the substructural characteristic they represent. Shown alongside the name of each key category are (1) the generic symbol used in the system for each category, and (2) the number of individual keys in each category. As the chart implies, the system permits probing in terms of gross structural features as well as in terms of substructural details in accord with the demands of individual queries.

TABLE I. CIDS STRUCTURAL SEARCH KEYS OVERVIEW



The individual keys in the several categories are displayed in subsequent sections of this report. Prefatorily, the reader is reminded that CIDS treats each bracketed part of a dot-connected structural formula of a compound as a separate structure. Recognition of this distinction between a "compound" and a "structure" is critical with respect to employment of the system.

2.1 MOLECULAR FORMULA COMPONENTS

CIDS provides for the search and retrieval of compounds on the basis of their complete molecular formula or any portion thereof. The precise molecular formula demands for retrieval are specified by either (or both) of two methods: the Molecular Formula Keys and the Molecular Formula Statement.

2.1.1 Molecular Formula (MF) Keys

The molecular formula keys enable the user to require the presence of a specified element in the total (Hill) molecular formula of all retrieved compounds. The system employs two types of molecular formula keys: (1) Quantitative, which specify the exact number of atoms of a particular element in the total molecular formula, and (2) Qualitative, which specify only that a particular element appears in the total molecular formula but do not specify the exact number of atoms.

CIDS provides specific molecular formula keys for deuterium and tritium, since the symbols for these isotopes (D and T, resp.) are included in the total molecular formula. (The molecular formula keys for H thus refer to natural hydrogen.)

In addition to the MF keys for the individual elements, CIDS defines the General Metal (MF) Key. This qualitative key is used to require that the total formula contain at least one atom of any metal. (A metal is defined in CIDS to mean any element except H, B, C, Si, N, P, As, Sb, O, S, Se, Te, F, Cl, Br, or I.)

Because of their high frequency of occurrence in organic compounds, nitrogen and oxygen are awarded quantitative keys for exactly zero atoms, thus making retrieval readily feasible on the basis of the absence of either or both of these elements in the total molecular formula. The absence of any other hetero-element is specified in the query by stipulating that the qualitative key for that heteroelement has not been assigned.

Table II. summarizes the molecular formula keys in the system.

TABLE II. CIDS MOLECULAR FORMULA KEYS

	Quantitative		Qualitative
Element	Number of atoms = 0	Number of atoms = 1,2,3,...	Number of atoms not specified
C		√	
H		√	
N	√	√	
O	√	√	
P		√	√
S		√	√
F		√	√
Cl		√	√
Br		√	√
I		√	√
Si		√	√
B		√	√
D (deuterium)			√
T (tritium)			√
All others			√
M (any metal)			√

The CIDS codes for the molecular formula keys are as follows:

Key type	Code (general form)*	Examples
Quantitative	MF El n	MF C 12 MF N 0 MF Si 2 MF C 1
Qualitative	MF El	MF Ag MF Si MF V MF T MF M

* El represents the element symbol
n represents the exact number of atoms

2.1.2 Molecular Formula Statement

While a Molecular Formula Key stipulates only the qualitative or quantitative presence of a particular element, the Molecular Formula Statement permits imposing the following kinds of restrictions:

1. The element types which appear in the molecular formula may be limited to those which are specifically enumerated in the Formula Statement.
2. The exact count, an upper and/or lower bound, or simply the qualitative presence of <u>any</u> element, including D and T, or of the general halogen symbol X (which represents any and all of the halogens F, Cl, Br, I) can be specified.
3. An algebraic relationship between the counts of any two elements in the molecular formula may be specified, provided this relationship takes the general form

$$El_1 = a\ El_2 \pm b$$

where El is the count of the element
a = 1,2,3...
b = 0,1,2...

Any of the above restrictions may be imposed on a total molecular formula, on one or more parts of a dot connected (addend) molecular formula, or on both.

2.2 STRUCTURAL FRAGMENT COMPONENTS

The term "structural fragment components" embraces all search keys which are automatically assigned to chemicals through computer examination of the node-connector representation of their structural formulas. It also embraces the Inorganic Compound Key (Section 2.2.11.1), which is actually assigned on the basis of an <u>absence</u> of a structural formula, and the Compound Class Keys (Section 2.2.11.6), none of which are currently in the system and some of which are envisioned as being assigned intellectually.

These components subdivide conveniently into rather conventional chemical categories and are so presented in the ensuing subsections of Section 2.2. The ordering of the categories is not intended to bear any relation to the order in which keys are either (a) assigned by the computer or (b) specified in the formulation of queries. Additional descriptive material is provided as it becomes appropriate to the various categories.

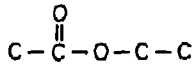
Special attention is directed to the fact that CIDS does NOT take into account the multiplying effect of numerical subscripts following brackets in arriving at the number of times a given fragment is present.

2.2.1 Acyclic-Cyclic (A-C) Key

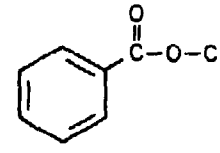
This single key operates to distinguish between organic compounds which are completely acyclic and those which are not.

Code	Description
A-C=n	Number (n) of rings* actually drawn† in structuring the total compound. (Rings within a bracketed, subscripted structure are counted only once.) For acyclic compounds, n = zero For cyclic compounds, n ≠ zero

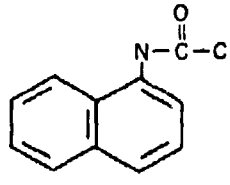
Examples, with A-C key codes:



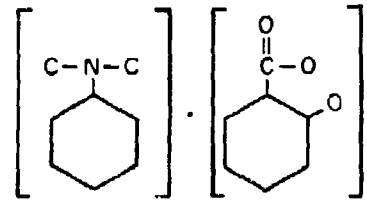
Example 1. A-C=0



Example 2. A-C=1



Example 3. A-C=2



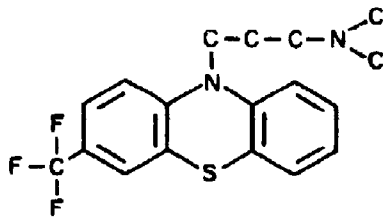
Example 4. A-C=2

---

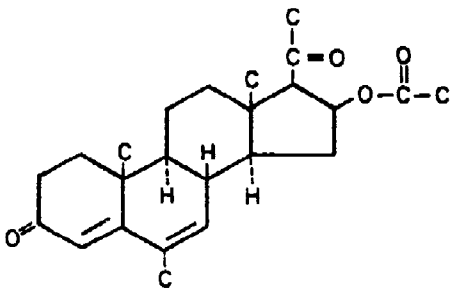
* The term "ring" means any individual closed chain of atoms. It is to be distinguished from the term "cyclic nucleus" which may consist of one or more rings.

Example: Each of the following---benzene, naphthalene, and anthracene--- is a single cyclic nucleus but the ring counts are, respectively, 1, 2, and 3.

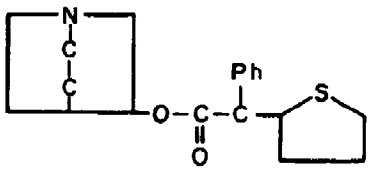
† The symbol Ph, representing phenyl, counts as one ring.



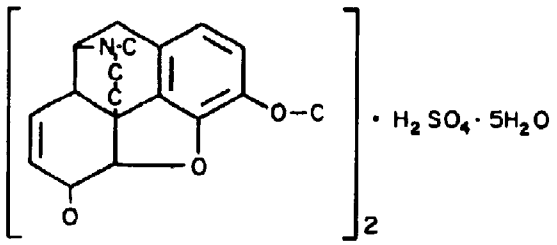
Example 5. A-C=3



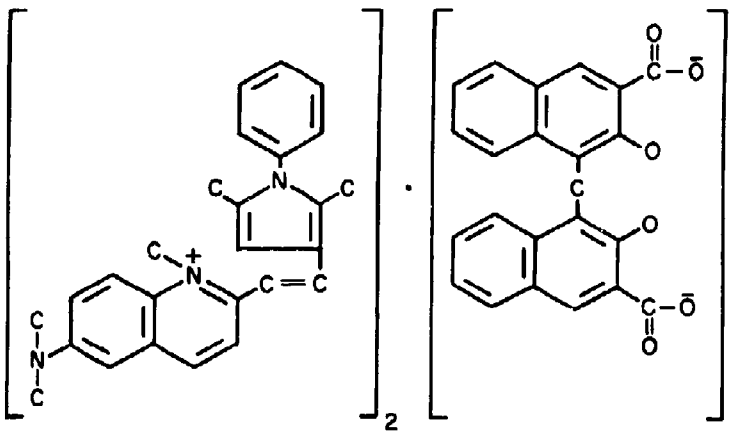
Example 6. A-C=4



Example 7. A-C=4



Example 8. A-C=5

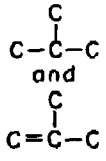
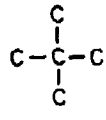


Example 9. A-C=8

2.2.2 Extracyclic (EC) Keys

Keys in this category describe the degree of saturation and the ⊥ and + configurations of the carbon atoms in all acyclic structures and in the acyclic portions of cyclic-acyclic structures.

TABLE III. EXTRACYCLIC (EC) KEYS

Formula	Code	Structure	Description
C_2	EC1=n	C=C	Total number (n) of extracyclic double bonds between C atoms regardless of any other attachments. If none, value assigned to n is zero. Either C may be in a cycle or the two may be in separate cycles.*
C_2	EC2=n	C≡C	Total number (n) of extracyclic triple bonds between C atoms regardless of any other attachments. If none, value assigned to n is zero.*
C_4	EC3=n		Total number (n) of completely acyclic ⊥ C configurations regardless of internal bonding or external connections. If none, value assigned to n is zero.**
C_5	EC4=n		Total number (n) of completely acyclic + C configurations regardless of external connections. If none, value assigned to n is zero.**

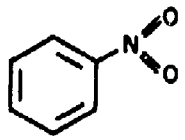
* If n=zero for both EC1 and EC2, the acyclic portion of the structure is saturated.

** If n=zero for both EC3 and EC4, the acyclic portion of the structure is normal (unbranched).

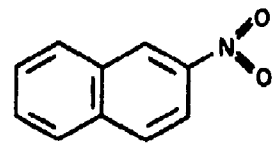
2.2.3 Number of Cyclic Nuclei (NCN) Key

Code	Description
NCN=n	Total number (n) of cyclic nuclei in the structure. If structure is acyclic, n = zero

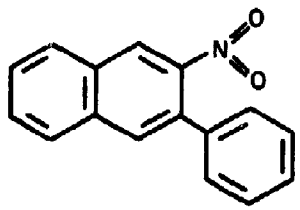
Examples, with NCN key codes:



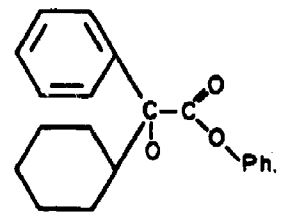
Example 1. NCN=1



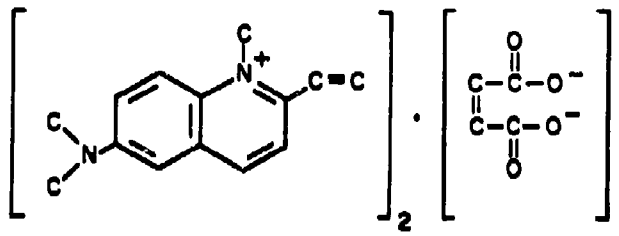
Example 2. NCN=1



Example 3. NCN=2



Example 4. NCN=3

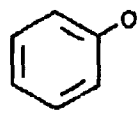


Example 5. NCN=1

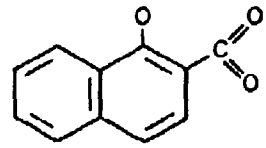
2.2.4 Cyclic Nuclei-Nonhydrogen Attachments (DACN) Key

Code	Description
DACN=n	Total number (n) of direct attachments between all cyclic nuclei of a structure and non-H atoms. Assigned only to structures containing one or more cyclic nuclei, i.e., to structure for which NCN≠0 (page 16).

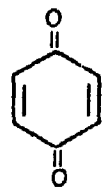
Examples, with the DACN key codes:



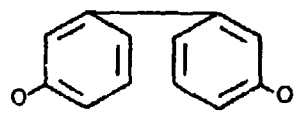
Example 1. DACN=1



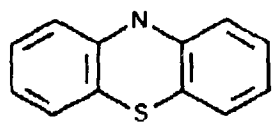
Example 2. DACN=2



Example 3. DACN=2



Example 4. DACN=4



Example 5. DACN=0

2.2.5 Generic Cyclic Nuclei (GCN) Keys

Keys in this category discriminate among cyclic nuclei in terms of the six structural characteristics identified in Table IV. The chemist will recognize these as features embodied in The Ring Index (2).

TABLE IV. GENERIC CYCLIC NUCLEI (GCN) KEYS

Class code	Key name	Description
GCN1	Ring Count	Smallest number of the smallest rings which will account for the entire nucleus
GCN2	Numerical Ring Population	Total number of atoms in each GCN1 ring of the nucleus
GCN3	Elementary Ring Population	Number of atoms of each element* in each GCN1 ring of the nucleus (Hill style)
GCN4	Skeleton Molecular Formula	Number of atoms of each element* in the entire nucleus (Hill style)
GCN5	Double Bond Count	Total number of double bonds in the entire nucleus
GCN6	Heteroelement distribution	Relative positions of heteroatoms in the nucleus. Assigned only to one-ring nuclei containing two or more heteroatoms† and a total of not more than fifteen atoms.

* The following elements are specified by their chemical symbols: Al, As, B, Bi, C, Ge, Hg, N, O, P, Pb, S, Sb, Se, Si, Sn, Te, and X (any halogen). Any other element is represented by the general symbol UH (unusual heteroelement).

† Throughout this handbook, the term "heteroatom" means one atom of any element other than carbon or hydrogen.

Assignment of the GCN1 through GCN5 keys to an assortment of cyclic nuclei is illustrated below. The chemical values and the complete CIDS codes are listed beneath each structure. One-ring nuclei are illustrated by Examples 1 through 4, two-ring nuclei by Examples 5 through 10, and polyring nuclei by Examples 11 and 12. Except for the GCN3 key, a single code for each key describes the entire nucleus. A GCN3 code is shown for each ring in a nucleus, except that a multiplier is used in lieu of repeating the code for identical rings, as illustrated by Examples 5, 6, 11, and 12. Coding of unusual heteroatoms (UH) is

illustrated in Example 10.

The GCN6 key is more involved in character but limited in scope, and illustrations of its assignment are therefore provided separately, immediately following these.

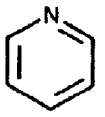
Examples:

Example 1

Value	Code
1	GCN1=1
6	GCN2=6
C_6	GCN3=C6
C_6	GCN4=C6
3	GCN5=3

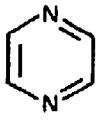
Example 2

Value	Code
1	GCN1=1
6	GCN2=6
C_6	GCN3=C6
C_6	GCN4=C6
0	GCN5=0



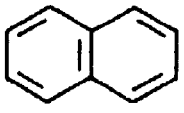
Example 3

Value	Code
1	GCN1=1
6	GCN2=6
C_5N	GCN3=C5 N1
C_5N	GCN4=C5 N1
3	GCN5=3



Example 4

Value	Code
1	GCN1=1
6	GCN2=6
C_4N_2	GCN3=C4 N2
C_4N_2	GCN4=C4 N2
3	GCN5=3

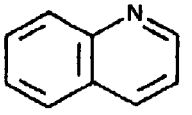


Example 5

Value	Code
2	GCN1=2
6,6	GCN2=6,6
C_6-C_6	GCN3=C6 (2)
C_{10}	GCN4=C10
5	GCN5=5

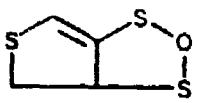
Example 6

Value	Code
2	GCN1=2
6,6	GCN2=6,6
C_6-C_6	GCN3=C6 (2)
C_{11}	GCN4=C11
0	GCN5=0



Example 7

Value	Code
2	GCN1=2
6,6	GCN2=6,6
C_5N-C_6	GCN3=C5 N1 GCN3=C6
C_9N	GCN4=C9 N1
5	GCN5=5

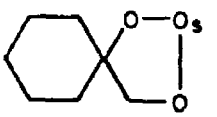


Example 8

Value	Code
2	GCN1=2
5,5	GCN2=5,5
C_2OS_2-C_4S	GCN3=C2 O1 S2 GCN3=C4 S1
C_4OS_3	GCN4=C4 O1 S3
1	GCN5=1

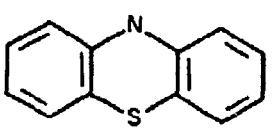
Example 9

Value	Code
2	GCN1=2
4,5	GCN2=4,5
C_3N-C_3NS	GCN3=C3 N1 GCN3=C3 N1 S1
C_5NS	GCN4=C5 N1 S1
0	GCN5=0



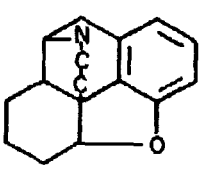
Example 10

Value	Code
2	GCN1=2
5,6	GCN2=5,6
C_2O_2Os-C_6	GCN3=C2 O2 UH1 GCN3=C_6
C_7O_2Os	GCN4=C7 O2 UH1
0	GCN5=0



Example 11

Value	Code
3	GCN1=3
6,6,6	GCN2=6,6,6
C_4NS-C_6-C_6	GCN3=C4 N1 S1 GCN3=C6 (2)
$C_{12}NS$	GCN4=C12 N1 S1
6	GCN5=6



Example 12

Value	Code
5	GCN1=5
5,6,6,6,6	GCN2=5,6,6,6,6
C_4O-C_5N-C_6-C_6-C_6	GCN3=C4 O1 GCN3=C5 N1 GCN3=C6 (3)
$C_{16}NO$	GCN4=C16 N1 O1
3	GCN5=3

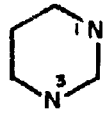
Assignment of the GCN6 keys is described and illustrated below:

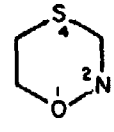
Heteroatoms in Ring	Locant 1	Citations of Locants in Code
Two or more, identical	Chosen so that the complete set of specified locants is the lowest possible set of numbers*	Ascending order
Two or more, all different	That atom which appears first in the sequence shown below.† (Direction of ring numbering is then chosen so that the complete set of specified locants is the lowest possible set of numbers*)	In the order of appearance in the sequence shown below†
Three or more, two or more of which are identical	That atom which (a) appears first in the sequence shown below† and (b) provides the lowest possible complete set of numbers*	In the order of appearance in the sequence shown below†

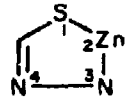
* Examples of lowest possible set of numbers: 1,2 is lower than 1,6; 1,3 is lower than 1,5; 1,2,4 is lower than 1,2,5; 1,2,5 is lower than either 1,3,4 or 1,3,6; 1,2,8,9 is lower than 1,3,4,10.

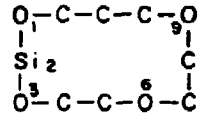
† Heteroatom Sequence: Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Hg, UH.

Examples‡, with GCN6 key codes:









‡ Structures are oriented arbitrarily as they might appear in the file compound.

2.2.6 Specific Cyclic Nuclei (SCN) Keys

CIDS provides specific keys for those individual cyclic nuclei which might be expected to occur with relatively high frequency in a large unbiased file of compounds. This provision, of course, is in addition to the generic keys (Sec. 2.2.5) for the same nuclei. The presence of the specific keys enhances practical utility by:

(a) permitting rapid retrieval of each such nucleus by means of a single key instead of by its collection of generic keys, and

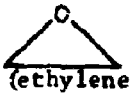
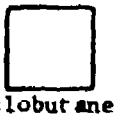
(b) prohibiting retrieval of each such nucleus when the search involves other nuclei in the same generic class.

The specific cyclic nuclei keys presently in the system are presented in Table V*. An oval within a ring signifies that that ring contains the maximum number of noncumulative double bonds and that it matters not which are shown as single and which as double. The Table can be updated through additions and deletions in accord with the dictates of experience.

An index to the nuclei through nomenclature is provided in Table VI, page 41.

* Ordering in the table is by the conventional method employed in The Ring Index and Chemical Abstracts.

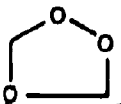
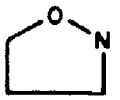
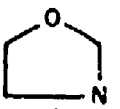
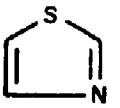
TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS*

SCN Code	Numerical Ring Population (GCN2)	Elementary Ring Population (GCN3)	Skeleton Molecular Formula (GCN4)	Structural Formula and Name
SCN1	3	C_2N	C_2N	 aziridine
SCN2	3	C_2O	C_2O	 oxirane (ethylene oxide)
SCN3	3	C_3	C_3	 cyclopropane
SCN4	4	C_4	C_4	 cyclobutane
SCN5	5	CN_4	CN_4	 1H-tetrazole
SCN6	5	C_2N_2O	C_2N_2O	 furazan
SCN7	5	C_2N_2S	C_2N_2S	 1,3,4-thiadiazole

* Ordering is by the conventional method employed in The Ring Index and Chemical Abstracts.

(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN8	5	C_2N_2S	C_2N_2S	 1,3,4-thiadiazoline
SCN9	5	C_2O_3	C_2O_3	 1,2,4-trioxolane
SCN10	5	C_3NO	C_3NO	 isoxazole
SCN11	5	C_3NO	C_3NO	 isoxazolidine
SCN12	5	C_3NO	C_3NO	 oxazole
SCN13	5	C_3NO	C_3NO	 oxazolidine
SCN14	5	C_3NS	C_3NS	 isothiazole
SCN15	5	C_3NS	C_3NS	 thiazole

(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN16	5	C_3NS	C_3NS	 thiazolidine
SCN17	5	C_3N_2	C_3N_2	 pyrazole
SCN18	5	C_3N_2	C_3N_2	 2-pyrazoline
SCN19	5	C_3N_2	C_3N_2	 pyrazolidine
SCN20	5	C_3N_2	C_3N_2	 imidazole
SCN21	5	C_3N_2	C_3N_2	 2-imidazoline
SCN22	5	C_3N_2	C_3N_2	 4-imidazoline
SCN23	5	C_3N_2	C_3N_2	 imidazolidine

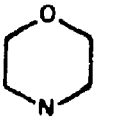
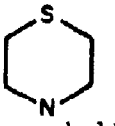
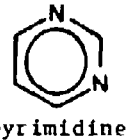
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN24	5	C_3O_2	C_3O_2	 1,3-dioxole
SCN25	5	C_4N	C_4N	 pyrrole
SCN26	5	C_4N	C_4N	 pyrrolidine
SCN27	5	C_4O	C_4O	 furan
SCN28	5	C_4O	C_4O	 tetrahydrofuran
SCN29	5	C_4S	C_4S	 thiophene
SCN30	5	C_4S	C_4S	 tetrahydrothiophene
SCN31	5	C_5	C_5	 cyclopentane

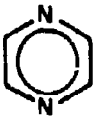
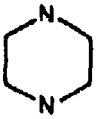
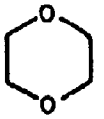
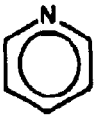
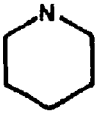
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN32	5	C_5	C_5	 cyclopentene
SCN33	5	C_5	C_5	 cyclopentadiene
SCN34	6	C_3N_3	C_3N_3	 s-triazine
SCN35	6	C_4NO	C_4NO	 morpholine
SCN36	6	C_4NS	C_4NS	 thiomorpholine
SCN37	6	C_4N_2	C_4N_2	 pyridazine
SCN38	6	C_4N_2	C_4N_2	 pyrimidine
SCN39	6	C_4N_2	C_4N_2	 1,2,3,4,-tetrahydropyrimidine

(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN40	6	C_4N_2	C_4N_2	 hexahydropyrimidine
SCN41	6	C_4N_2	C_4N_2	 pyrazine
SCN42	6	C_4N_2	C_4N_2	 piperazine
SCN43	6	C_4O_2	C_4O_2	 1,4-dioxane
SCN44	6	C_5N	C_5N	 pyridine
SCN45	6	C_5N	C_5N	 piperidine
SCN46	6	C_5O	C_5O	 4H-pyran
SCN47	6	C_5O	C_5O	 tetrahydropyran

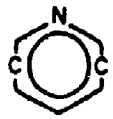
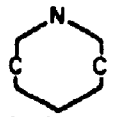
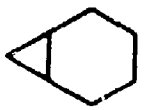
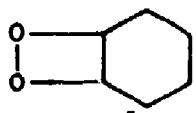
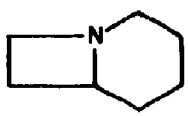
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN48	6	C_6	C_6	 benzene
SCN49	6	C_6	C_6	 cyclohexane
SCN50	6	C_6	C_6	 cyclohexene
SCN51	6	C_6	C_6	 1,3-cyclohexadiene
SCN52	6	C_6	C_6	 1,4-cyclohexadiene
SCN53	7	C_6N	C_6N	 hexahydroazepine (hexamethylenimine)
SCN54	7	C_7	C_7	 cycloheptane
SCN55	7	C_7	C_7	 cycloheptene

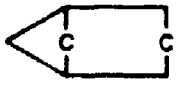
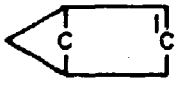
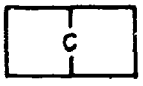
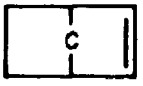
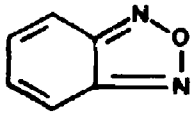
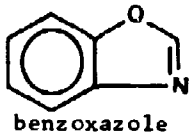
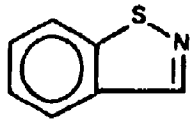
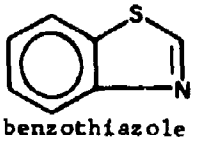
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN56	7	C_7	C_7	 1,3,5-cycloheptatriene
SCN57	8	C_7N	C_7N	 azocine
SCN58	8	C_7N	C_7N	 octahydroazocine
SCN59	8	C_8	C_8	 cyclooctane
SCN60	3,6	C_3-C_6	C_7	 norcarane
SCN61	4,5	C_3N-C_3NS	C_5NS	 4-thia-1-azabicyclo[3.2.0]-heptane
SCN62	4,6	C_2O_2-C_6	C_6O_2	 7,8-dioxabicyclo[4.2.0]octane
SCN63	4,6	C_3N-C_5N	C_7N	 conidine

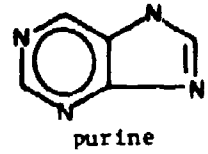
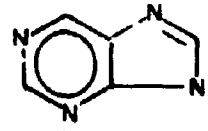
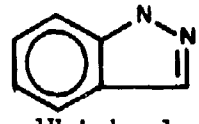
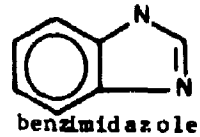
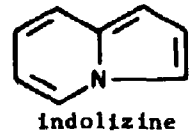
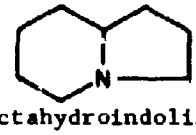
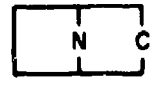
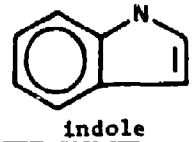
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN64	4,6	C_4-C_6	C_7	 norpinane
SCN65	4,6	C_4-C_6	C_7	 2-norpinene
SCN66	5,5	C_5-C_5	C_7	 norbornane
SCN67	5,5	C_5-C_5	C_7	 2-norbornene
SCN68	5,6	C_2N_2O-C_6	C_6N_2O	 benzofurazan
SCN69	5,6	C_3NO-C_6	C_7NO	 benzoxazole
SCN70	5,6	C_3NS-C_6	C_7NS	 1,2-benzisothiazole
SCN71	5,6	C_3NS-C_6	C_7NS	 benzothiazole

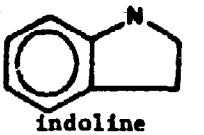
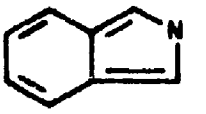
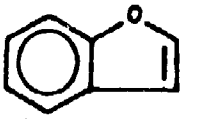
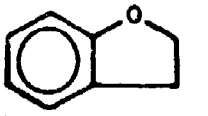
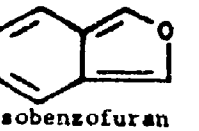
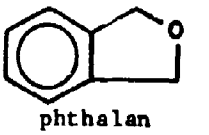
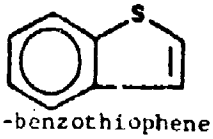
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN72	5,6	C_3N_2-C_4N_2	C_5N_4	 purine
SCN73	5,6	C_3N_2-C_4N_2	C_5N_4	 9H-purine
SCN74	5,6	C_3N_2-C_6	C_7N_2	 1H-indazole
SCN75	5,6	C_3N_2-C_6	C_7N_2	 benzimidazole
SCN76	5,6	C_4N-C_5N	C_8N	 indolizine
SCN77	5,6	C_4N-C_5N	C_8N	 octahydroindolizine
SCN78	5,6	C_4N-C_5N	C_7N	 nortropane
SCN79	5,6	C_4N-C_6	C_8N	 indole

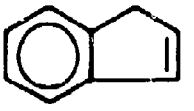
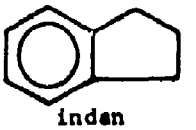
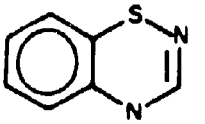
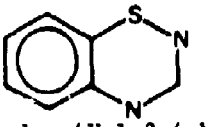
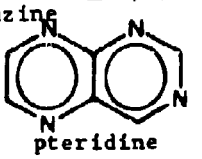
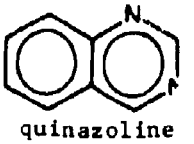
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN80	5,6	C_4N-C_6	C_8N	 indoline
SCN81	5,6	C_4N-C_6	C_8N	 isoindole
SCN82	5,6	C_4N-C_6	C_8N	 isoindoline
SCN83	5,6	C_4O-C_6	C_8O	 benzofuran
SCN84	5,6	C_4O-C_6	C_8O	 2,3-dihydrobenzofuran
SCN85	5,6	C_4O-C_6	C_8O	 isobenzofuran
SCN86	5,6	C_4O-C_6	C_8O	 phthalan
SCN87	5,6	C_4S-C_6	C_8S	 1-benzothiophene

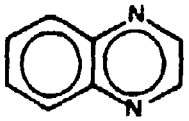
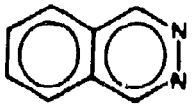
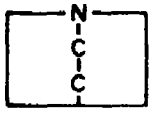
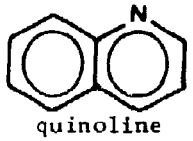
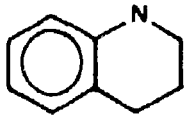
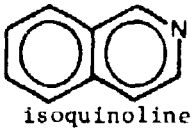
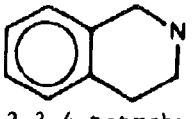
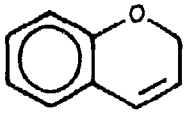
(continued)

TABLE V. SPECIFIC CYCLIC NUCLE. (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN88	5,6	C_5-C_6	C_9	 indene
SCN89	5,6	C_5-C_6	C_9	 indan
SCN90	5,7	C_5-C_7	C_{10}	 azulene
SCN91	6,6	C_3N_2S-C_6	C_7N_2S	 4H-1,2,4-benzothiadiazine
SCN92	6,6	C_3N_2S-C_6	C_7N_2S	 2,3-dihydro-4H-1,2,4-benzothiadiazine
SCN93	6,6	C_4N_2-C_4N_2	C_6N_4	 pteridine
SCN94	6,6	C_4N_2-C_6	C_8N_2	 cinnoline
SCN95	6,6	C_4N_2-C_6	C_8N_2	 quinazoline

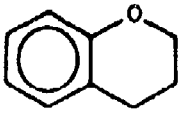
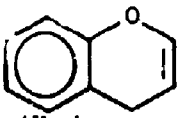
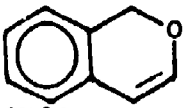
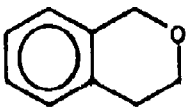
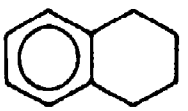
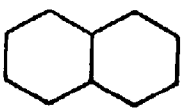
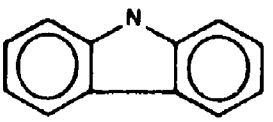
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN96	6,6	C_4N_2-C_6	C_8N_2	 quinoxaline
SCN97	6,6	C_4N_2-C_6	C_8N_2	 phthalazine
SCN98	6,6	C_5N-C_5N	C_7N	 quinuclidine
SCN99	6,6	C_5N-C_6	C_9N	 quinoline
SCN100	6,6	C_5N-C_6	C_9N	 1,2,3,4-tetrahydroquinoline
SCN101	6,6	C_5N-C_6	C_9N	 isoquinoline
SCN102	6,6	C_5N-C_6	C_9N	 1,2,3,4-tetrahydro-isoquinoline
SCN103	6,6	C_5O-C_6	C_9O	 2H-chromene

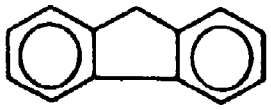
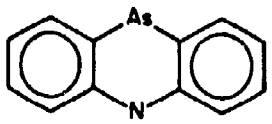
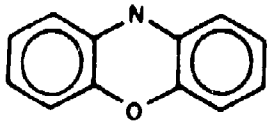
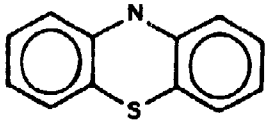
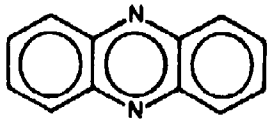
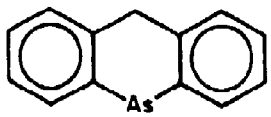
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN104	6,6	C_5O-C_6	C_9O	 chroman
SCN105	6,6	C_5O-C_6	C_9O	 4H-chromene
SCN106	6,6	C_5O-C_6	C_9O	 1H-2-benzopyran
SCN107	6,6	C_5O-C_6	C_9O	 isochroman
SCN108	6,6	C_6-C_6	C_{10}	 naphthalene
SCN109	6,6	C_6-C_6	C_{10}	 1,2,3,4-tetrahydronaphthalene
SCN110	6,6	C_6-C_6	C_{10}	 decalin
SCN111	5,6,6	C_4N-C_6-C_6	$C_{12}N$	 carbazole

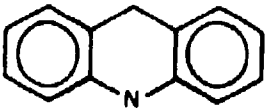
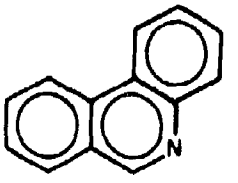
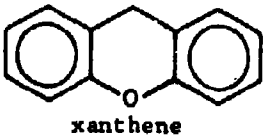
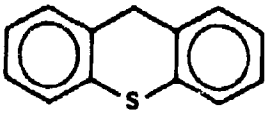
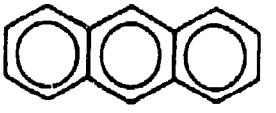
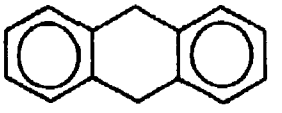
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN112	5,6,6	C_5-C_6-C_6	C_{13}	 fluorene
SCN113	5,6,6	C_5-C_6-C_6	C_{12}	 acenaphthene
SCN114	6,6,6	C_4AsN-C_6-C_6	$C_{12}AsN$	 5,10-dihydrophenarsazine
SCN115	6,6,6	C_4NO-C_6-C_6	$C_{12}NO$	 phenoxazine
SCN116	6,6,6	C_4NS-C_6-C_6	$C_{12}NS$	 phenothiazine
SCN117	6,6,6	C_4N_2-C_6-C_6	$C_{12}N_2$	 phenazine
SCN118	6,6,6	C_5As-C_6-C_6	$C_{13}As$	 5,10-dihydroacridarsine

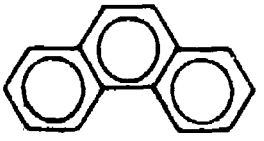
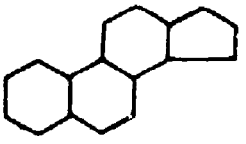
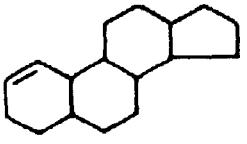
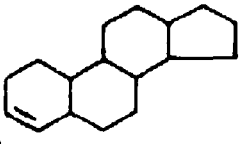
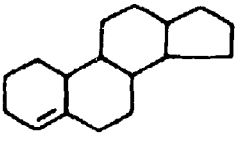
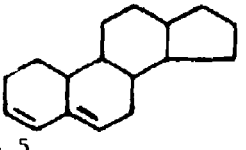
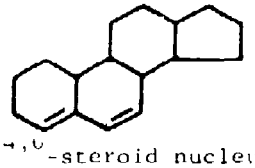
(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN119	6,6,6	C_5N-C_6-C_6	$C_{13}N$	 acridine.
SCN120	6,6,6	C_5N-C_6-C_6	$C_{13}N$	 acridan
SCN121	6,6,6	C_5N-C_6-C_6	$C_{13}N$	 phenanthridine
SCN122	6,6,6	C_5O-C_6-C_6	$C_{13}O$	 xanthene
SCN123	6,6,6	C_5S-C_6-C_6	$C_{13}S$	 thioxanthene
SCN124	6,6,6	C_6-C_6-C_6	C_{14}	 anthracene
SCN125	6,6,6	C_6-C_6-C_6	C_{14}	 dihydroanthracene

(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (continued)

SCN	GCN2	GCN3	GCN4	Structural Formula
SCN126	6,6,6	C_6-C_6-C_6	C_{14}	 phenanthrene
SCN127	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 saturated steroid nucleus
SCN128	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 Δ^1-steroid nucleus
SCN129	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 Δ^3-steroid nucleus
SCN130	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 Δ^4-steroid nucleus
SCN131	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 $\Delta^{3,5}$-steroid nucleus
SCN132	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 $\Delta^{3,6}$-steroid nucleus

(continued)

TABLE V. SPECIFIC CYCLIC NUCLEI (SCN) KEYS (concluded)

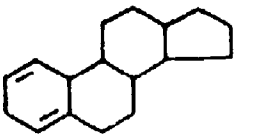
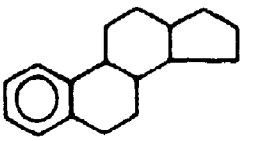
SCN	GCN2	GCN3	GCN4	Structural Formula
SCN133	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 $\Delta^{1,4}$-steroid nucleus
SCN134	5,6,6,6	C_5-C_6-C_6-C_6	C_{17}	 $\Delta^{1,3,5(10)}$-steroid nucleus

TABLE VI. SPECIFIC CYCLIC NUCLEI - NOMENCLATURE INDEX

Nucleus*	Ring Index Number	Code
Acenaphthene	3133	SCN113
Acridan	3523	SCN120
Acridine	3523	SCN119
Anthracene	3618	SCN124
Aziridine	11	SCN1
Azocine	414	SCN57
Azulene	1446	SCN90
Benzene	292	SCN48
Benzimidazole	1213	SCN75
1,2-Benzisothiazole	1150	SCN70
Benzofuran	1328	SCN83
Benzofurazan	1058	SCN68
1H-2-Benzopyran	1732	SCN106
4H-1,2,4-Benzothiadiazine	1515	SCN91
Benzothiazole	1152	SCN71
1-Benzothiophene	1353	SCN87
Benzoxazole	1125	SCN69
Carbazole	2927	SCN111
Chroman	1727	SCN104
2H-Chromene	1727	SCN103
4H-Chromene	1728	SCN105
Cinnoline	1625	SCN94
Conidine	810	SCN63
Cyclobutane	49	SCN4
Cycloheptane	361	SCN54
1,3,5-Cycloheptatriene	361	SCN56
Cycloheptene	361	SCN55
1,3-Cyclohexadiene	293	SCN51
1,4-Cyclohexadiene	293	SCN52
Cyclohexane	293	SCN49

* Preferred Ring Index names.

(Continued)

TABLE VI. SPECIFIC CYCLIC NUCLEI - NOMENCLATURE INDEX (Continued)

Nucleus	Ring Index Number	Code
Cyclohexene	293	SCN50
Cyclooctane	417	SCN59
Cyclopentadiene	155	SCN33
Cyclopentane	155	SCN31
Cyclopentene	155	SCN32
Cyclopropane	14	SCN3
Decalin	1754	SCN110
5,10-Dihydroacridarsine	3454	SCN118
Dihydroanthracene	3618	SCN125
2,3-Dihydrobenzofuran	1328	SCN84
2,3-Dihydro-4H-1,2,4-benzothiadiazine	1515	SCN92
5,10-Dihydrophenarsazine	3257	SCN114
7,8-Dioxabicyclo 4.2.0 octane	806	SCN62
1,4-Dioxane	263	SCN43
1,3-Dioxole	136	SCN24
Ethylene Oxide	12	SCN2
Fluorene	3127	SCN112
Furan	145	SCN27
Furazan	84	SCN6
Hexahydroazepine	355	SCN53
Hexahydropyrimidine	249	SCN40
Hexamethylenimine	355	SCN53
Imidazole	127	SCN20
Imidazolidine	127	SCN23
2-Imidazoline	127	SCN21
4-Imidazoline	127	SCN22
Indan	1391	SCN89
1H-Indazole	1209	SCN74
Indene	1391	SCN88
Indole	1286	SCN79
Indoline	1286	SCN80

(Continued)

TABLE VI. SPECIFIC CYCLIC NUCLEI - NOMENCLATURE INDEX (Continued)

Nucleus	Ring Index Number	Code
Indolizine	1276	SCN76
Isobenzofuran	1330	SCN85
Isochroman	1732	SCN107
Isoindole	1290	SCN81
Isoindoline	1290	SCN82
Isoquinoline	1708	SCN101
Isothiazole	120	SCN14
Isoxazole	118	SCN10
Isoxazolidine	118	SCN11
Morpholine	239	SCN35
Naphthalene	1754	SCN108
Norbornane	1031	SCN66
2-Norbornene	1031	SCN67
Norcarane	722	SCN60
Norpinane	832	SCN64
2-Norpinene	832	SCN65
Nortropane	1281	SCN78
Octahydroazocine	414	SCN58
Octahydroindolizine	1276	SCN77
Oxazole	119	SCN12
Oxazolidine	119	SCN13
Oxirane	12	SCN2
Phenanthrene	3619	SCN126
Phenanthridine	3528	SCN121
Phenazine	3390	SCN117
Phenothiazine	3314	SCN116
Phenoxazine	3290	SCN115
Phthalan	1330	SCN86
Phthalazine	1628	SCN97
Piperazine	250	SCN42
Piperidine	277	SCN45

(Continued)

TABLE VI. SPECIFIC CYCLIC NUCLEI - NOMENCLATURE INDEX (Continued)

Nucleus	Ring Index Number	Code
Pteridine	1587	SCN93
Purine	1179	SCN72
9H-Purine	1180	SCN73
4H-Pyran	279	SCN46
Pyrazine	250	SCN41
Pyrazole	124	SCN17
Pyrazolidine	124	SCN19
2-Pyrazoline	124	SCN18
Pyridazine	248	SCN37
Pyridine	277	SCN44
Pyrimidine	249	SCN38
Pyrrole	142	SCN25
Pyrrolidine	142	SCN26
Quinazoline	1626	SCN95
Quinoline	1707	SCN99
Quinoxaline	1627	SCN96
Quinuclidine	1690	SCN98
Steroid nucleus, saturated	4781	SCN127
Δ^{1}-Steroid nucleus	4781	SCN128
$\Delta^{1,3,5(10)}$-Steroid nucleus	4781	SCN134
$\Delta^{1,4}$-Steroid nucleus	4781	SCN133
Δ^{3}-Steroid nucleus	4781	SCN129
$\Delta^{3,5}$-Steroid nucleus	4781	SCN131
Δ^{4}-Steroid nucleus	4781	SCN130
$\Delta^{4,6}$-Steroid nucleus	4781	SCN132
Tetrahydrofuran	145	SCN28
1,2,3,4-Tetrahydroisoquinoline	1708	SCN102
1,2,3,4-Tetrahydronaphthalene	1754	SCN109
Tetrahydropyran	278	SCN47
1,2,3,4-Tetrahydropyrimidine	249	SCN39
1,2,3,4-Tetrahydroquinoline	1707	SCN100
Tetrahydrothiophene	149	SCN30

(Continued)

TABLE VI. SPECIFIC CYCLIC NUCLEI - NOMENCLATURE INDEX (Concluded)

Nucleus	Ring Index Number	Code
1H-Tetrazole	61	SCN5
4-Thia-1-azabicyclo 3.2.0 heptane	774	SCN61
1,3,4-Thiadiazole	90	SCN7
1,3,4-Thiadiazoline	90	SCN8
Thiazole	122	SCN15
Thiazolidine	122	SCN16
Thiomorpholine	245	SCN36
Thiophene	149	SCN29
Thioxanthene	3607	SCN123
s-Triazine	212	SCN34
1,2,4-Trioxolane	111	SCN9
Xanthene	3571	SCN122

2.2.7 Specific Functional Group (FG) Keys

CIDS defines a functional group as a structured assemblage of atoms which is characteristic of a particular structural class of chemical compounds, e.g., ethers, carboxylic acids, sulfones, nitro compounds, etc. As with other structural fragment components, functional groups used as search tools in the system are represented by search keys. As would be expected, nearly all of the functional groups contain one or more heteroatoms; the exceptions are the three C_2 keys and the C_3 and C_4 keys, all of which represent specific states of extracyclic unsaturation (dehydrogenation).

A key point in the philosophy of CIDS consists of restricting the selection of specific functional group keys to those which are expected to occur with sufficiently high frequency in a large file of compounds to warrant their use as automatic tools for rapid structural differentiation. The present lexicon of these keys is displayed in Table VII where the ordering is by Hill molecular formula with the general heteroelement symbol, El, subordinate to any specific element symbols shown in the fragment. The lexicon is open ended in order that it may be updated periodically as may be desired.

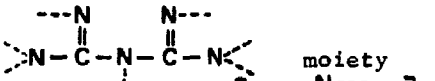
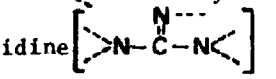
Additional explanatory notes concerning the structuring and use of specific functional group keys follow:

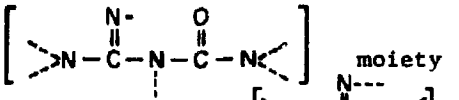
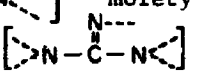
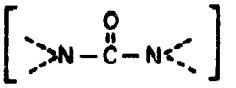
1. Fragments are assigned on the basis of total composition only. For example, a fragment of composition C_2O_2 is not assigned any key representing a fragment of lesser composition such as C_2O, CO_2, CO, C_2, O_2 or O. The only exception is in connection with FG23 [~C=El~], FG121 [~C≡C–El~], and FG122 [~El–C=C–El~]. With these, all specific functional group keys contained within (but not coinciding with) them are assigned in addition to them. In instances where the specific key and the El key coincide, the usual procedure of assigning only the specific key is followed.

2. In the assignment of fragments which are identical in all respects except the character of the hanging bond, the one with the solid line is superior to the one with the broken line which, in turn, is superior to the one with the wiggly line.

3. In the case of overlapping fragments in a structure (i.e., one or more of the atoms in one fragment functions also in an adjoining fragment) both fragments are assigned.

Examples:

(1) A compound containing an  moiety would receive an assignment of two guanidine  keys.

(2) A compound containing an  moiety would receive an assignment of one guanidine  and one urea  key.

4. In addition to the international chemical symbols for the elements, the following are employed in fragment portrayal:

X means any member of the halogen family (F, Cl, Br, I)

E means any heteroelement, i.e., any element except C and H

(E) means any element except C in a ring

5. All fragments which contain halogen atoms employ the general halogen symbol X. No fragments are employed which specify a particular halogen.

6. The lines in a fragment represent valence bonds in the broad sense, i.e., without regard to the physical or chemical character of the bonds. In the few instances where it is considered best practice, positive and negative charge signs are also employed.

7. Each fragment has one or more "hanging" (one end unattached) bonds to represent attachment to the rest of the structure. Three kinds of hanging bonds are used:

(a) Solid line (———) signifies a single bond attached at the open end to C.

(b) Broken line (- - - - - - -) signifies a single bond attached at the open end to either C or H.

(c) Wiggly line (~~~) signifies any kind of attachment, i.e., single or multiple bonding to any atom or atoms, or no attachment at all. Often referred to as a "don't care bond".

8. If the number of straight lines (solid plus broken) running from an uncharged atom is less than that stipulated in the following valence table, attachment(s) to the requisite number of H atoms to account for the difference is implied.

Atom	Valence
C, Si	4
B, N, P, As, Sb	3
O, S, Se, Te	2

9. No fragment begins or ends with a double or triple bond. A wiggly line representing an unspecified bond type, however, is employed.

10. Display of carbon as a component of the fragment is limited to instances in which its exclusion would wither violate (9) above or discriminate less specifically than desired.

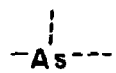
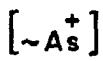
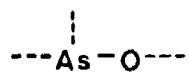
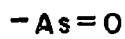
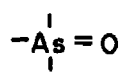
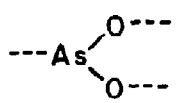
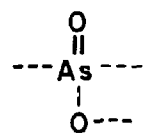
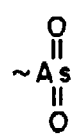
11. Except where specified in the fragment structure, no atom of the fragment can be part of a ring. However, wherever the fragment structure permits, the entire fragment may be attached either to an open chain atom or to a ring atom, and the search strategy distinguishes between these two attachments by appending the letter R to the code whenever the attachment is to a ring. In the case of a fragment having more than one hanging bond, the fragment is considered attached to a ring if any one of the attachments is to a ring.

12. An anion derived from a systematic organic acid is assigned the same key as the total acid. (By a systematic acid is meant any compound treated as an acid in IUPAC/CA systematic nomenclature, e.g., acetic acid, benzimidic acid, picric acid, etc.)

13. For the convenience of users who may wish on occasion to identify keys through a nomenclature approach, a name index to the specific functional groups represented in the system is provided in Table VIII, page 75.

14. The total list of specific functional group keys presented in Table VII is subdivided in tables IX through XXII in terms of the individual heteroatoms contained in the groups.

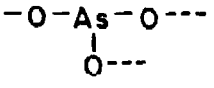
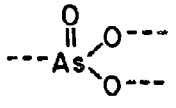
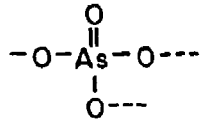
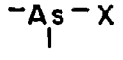
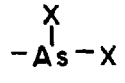
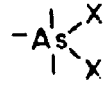
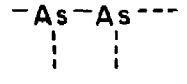
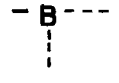
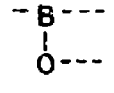
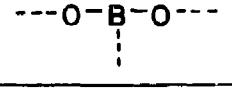
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS

Code*	Formula	Structure	User's notes
FG1	Ag		
FG2	Al		
FG3	As		
FG4			
FG5	AsO		
FG6			
FG7			
FG8	AsO_2		
FG9			
FG10			

(continued)

* The letter R is appended to the code whenever one or more of the fragment attachments is to a ring atom.

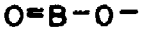
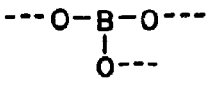
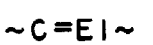
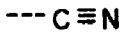
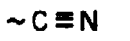
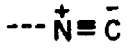
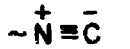
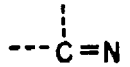
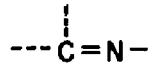
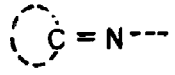
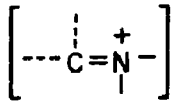
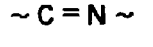
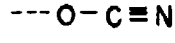
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG11	AsO_3		
FG12			
FG13	AsO_4		
FG14	AsX		
FG15	AsX_2		
FG16			
FG17	As_2		
FG18	B		
FG19	BO		
FG20	BO_2		

* See page 49.

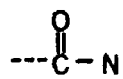
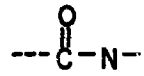
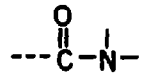
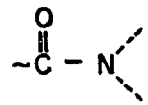
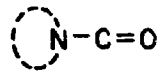
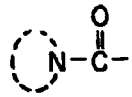
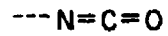
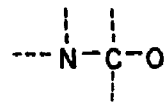
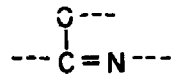
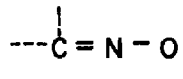
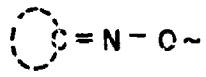
(continued)

TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG21	BO_2		
FG22	BO_3		
FG23	CEl		Caution! See explanatory note 1, p. 46.
FG24	CN		
FG25			
FG26			
FG27			
FG28			
FG29			
FG30			
FG31			
FG32			
FG33	CNO		

* See page 49. (continued)

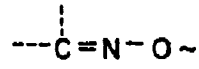
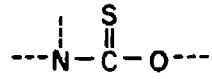
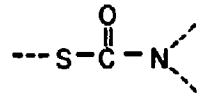
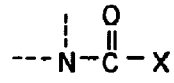
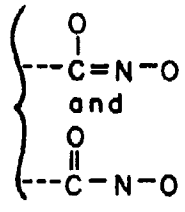
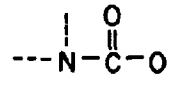
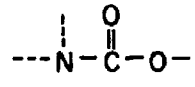
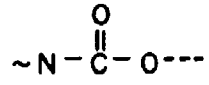
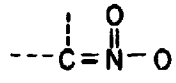
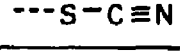
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG34	CNO		
FG35			
FG36			
FG37			
FG38			
FG39			
FG40			
FG41			
FG42			
FG43			
FG44			

* See page 49.

(continued)

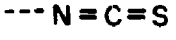
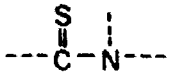
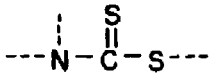
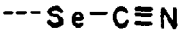
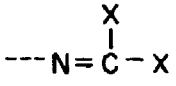
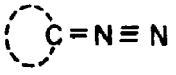
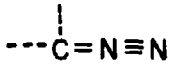
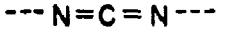
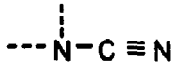
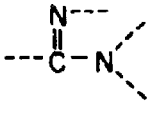
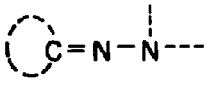
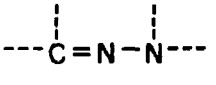
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG45	CNO		
FG46	CNOS		
FG47			
FG48	CNOX		
FG49	CNO_2		
FG50			
FG51			
FG52			
FG53			
FG54	CNS		

* See page 49.

(continued)

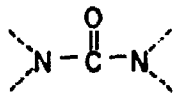
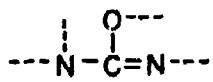
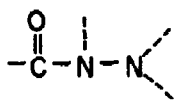
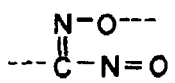
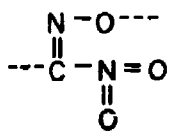
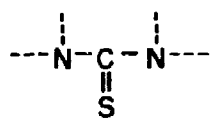
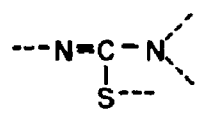
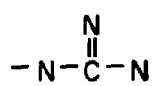
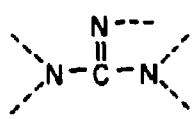
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG55	CNS		
FG56			
FG57	CNS_2		
FG58	CNSe		
FG59	CNX_2		
FG60	CN_2		
FG61			
FG62			
FG63			
FG64			
FG65			
FG66			

* See page 49.

(continued)

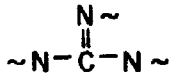
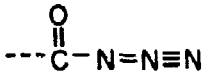
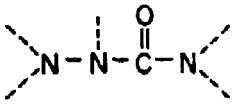
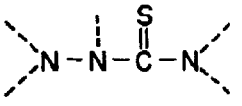
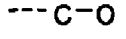
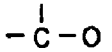
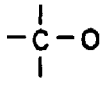
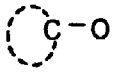
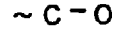
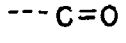
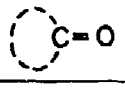
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG67	CN_2O		
FG68			
FG69			
FG70	CN_2O_2		
FG71	CN_2O_3		
FG72	CN_2S		
FG73			
FG74	CN_3		
FG75			

* See page 49.

(continued)

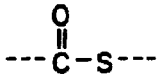
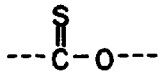
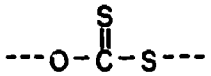
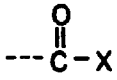
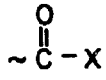
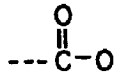
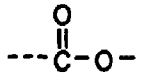
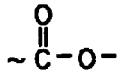
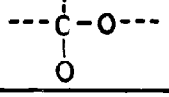
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG76	CN_3		
FG77	CN_3O		
FG78			
FG79	CN_3S		
FG80	CO		
FG81			
FG82			
FG83			
FG84			
FG85			
FG86			
FG87			

* See page 49.

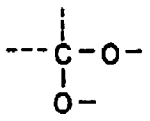
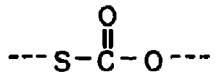
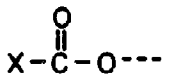
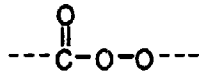
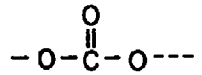
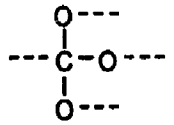
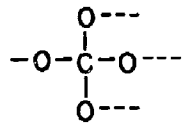
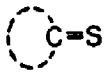
(continued)

TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG88	CO		
FG89	COS		
FG90			
FG91	COS_2		
FG92	COX		
FG93			
FG94	CO_2		
FG95			
FG96			
FG97			
FG98			

* See page 49. (continued)

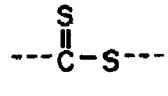
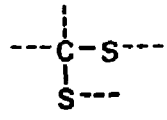
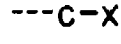
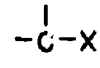
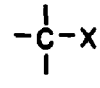
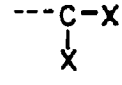
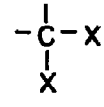
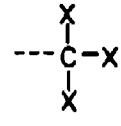
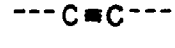
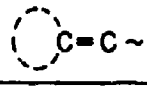
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FC) KEYS (continued)

Code*	Formula	Structure	User's notes
FG99	CO_2		
FG100	CO_2S		
FG101	CO_2X		
FG102	CO_3		
FG103			
FG104			
FG105	CO_4		
FG106	CS		
FG107			
FG108			

* See page 49.

(continued)

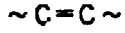
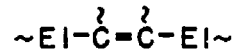
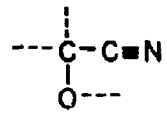
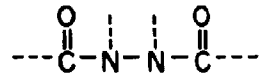
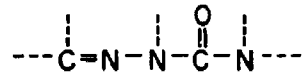
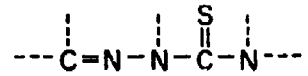
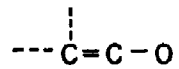
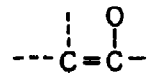
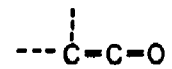
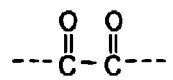
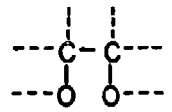
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG109	CS		
FG110	CS_2		
FG111			
FG112	CX		
FG113			
FG114			
FG115	CX_2		
FG116			
FG117	CX_3		
FG118	C_2		
FG119			

* See page 49.

(continued)

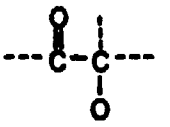
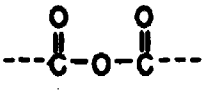
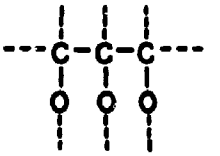
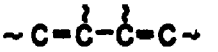
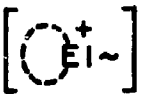
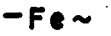
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG120	C_2		
FG121	C_2El		Caution! See explanatory note 1, p. 46.
FG122	C_2El_2		Caution! See explanatory note 1, p 46
FG123	C_2NO		
FG124	$C_2N_2O_2$		
FG125	C_2N_3O		
FG126	C_2N_3S		
FG127	C_2O		
FG128			
FG129			
FG130	C_2O_2		
FG131			

* See page 49.

(continued)

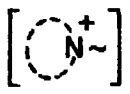
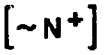
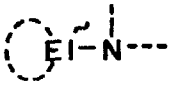
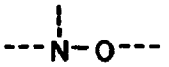
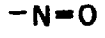
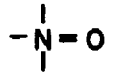
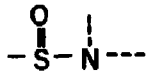
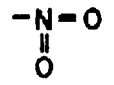
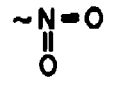
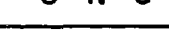
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG132	C_2O_2		
FG133	C_2O_3		
FG134	C_3		
FG135	C_3O_3		
FG136	C_4		
FG137	El		
FG138	Fe		
FG139	Hg		
FG140	K		
FG141	Li		
FG142	Mg		
FG143	N		

* See page 49.

(continued)

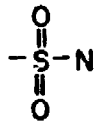
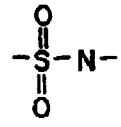
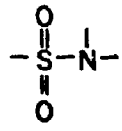
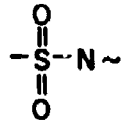
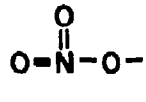
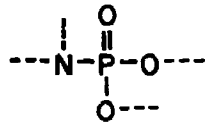
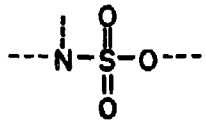
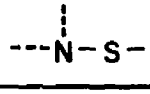
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG144	N		
FG145			
FG146			
FG147			
FG148	NE1		
FG149	NO		
FG150			
FG151			
FG152			
FG153	NOS		
FG154	NO_2		
FG155			
FG156			

(continued)

* See page 49.

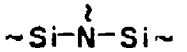
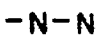
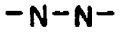
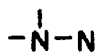
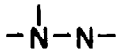
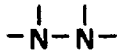
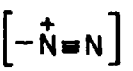
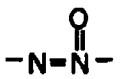
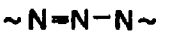
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG157	NO_2S		
FG158			
FG159			
FG160			
FG161	NO_3		
FG162	NO_3P		
FG163	NO_3S		
FG164	NP		
FG165	NS		

* See page 49.

(continued)

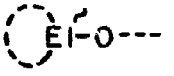
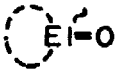
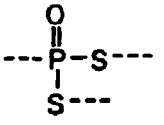
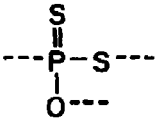
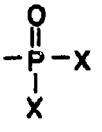
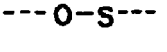
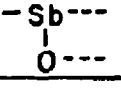
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG166	NSi_2		
FG167	N_2		
FG168			
FG169			
FG170			
FG171			
FG172			
FG173			
FG174	N_2O		
FG175	N_3		
FG176			
FG177	Na		
FG178	O		
FG179			

* See page 49.

(continued)

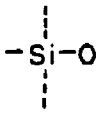
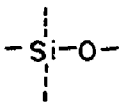
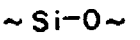
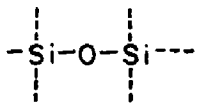
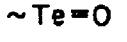
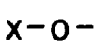
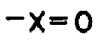
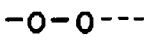
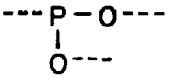
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG180	OE1		
FG181			
FG182	OP		
FG183	OPS_2		
FG184			
FG185	OPX_2		
FG186	OS		
FG187			
FG188	OSX		
FG189	OSb		

* See page 49.

(continued)

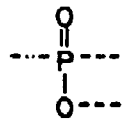
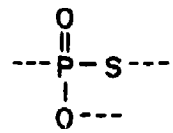
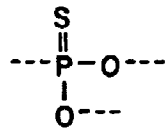
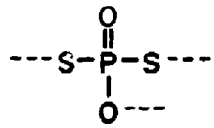
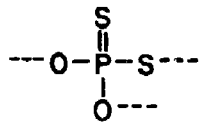
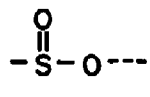
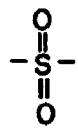
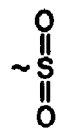
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG190	OSb		
FG191	OSe		
FG192	OSi		
FG193			
FG194			
FG195	OSi_2		
FG196	OTe		
FG197	OX		
FG198			
FG199	O_2		
FG200	O_2P		

* See page 49.

(continued)

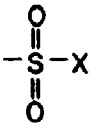
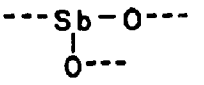
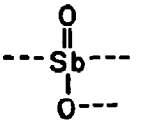
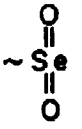
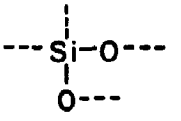
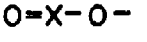
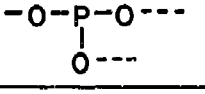
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG201	O_2P		
FG202	O_2PS		
FG203			
FG204	O_2PS_2		
FG205			
FG206	O_2S		
FG207			
FG208			

* See page 49.

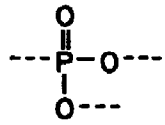
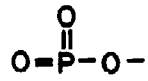
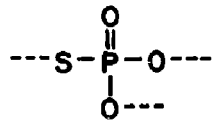
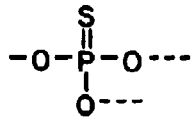
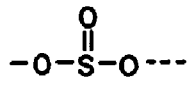
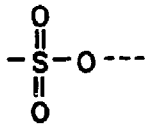
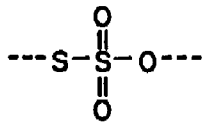
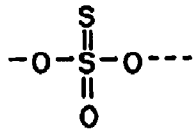
(continued)

TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG209	O_2SX		
FG210	O_2Sb		
FG211			
FG212	O_2Se		
FG213	O_2Si		
FG214	O_2Te		
FG215	O_2X		
FG216			
FG217	O_3P		

* See page 79. (continued)

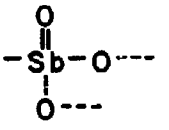
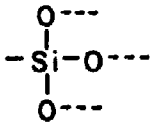
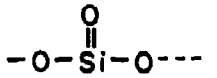
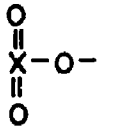
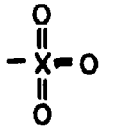
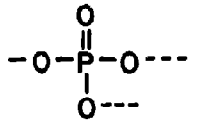
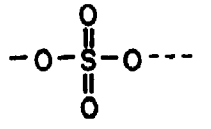
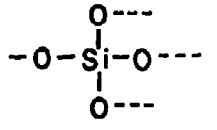
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG218	O_3P		
FG219			
FG220	O_3PS		
FG221			
FG222	O_3S		
FG223			
FG224	O_3S_2		
FG225			

* See page 49.

(continued)

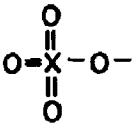
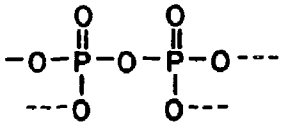
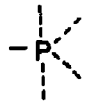
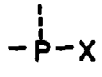
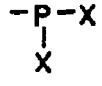
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG226	O_3Sb		
FG227	O_3Si		
FG228			
FG229	O_3X		
FG230			
FG231	O_4P		
FG232	O_4S		
FG233	O_4Si		

* See page 49.

(continued)

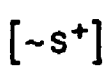
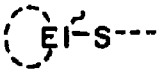
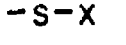
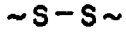
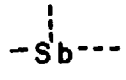
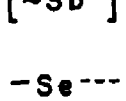
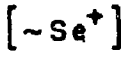
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG234	O_4X		
FG235	O_7P_2		
FG236	P		
FG237			
FG238			
FG239			
FG240			
FG241	PX		
FG242	PX_2		
FG243	P_2		
FG244	Pb		
FG245	S		

* See page 49.

(continued)

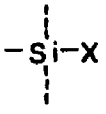
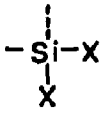
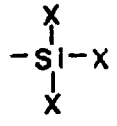
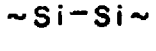
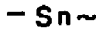
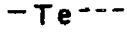
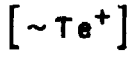
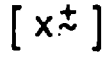
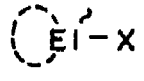
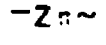
TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (continued)

Code*	Formula	Structure	User's notes
FG246	S		
FG247			
FG248	SEl		
FG249			
FG250	SX		
FG251	S_2		
FG252	Sb		
FG253			
FG254	Se		
FG255			
FG256	Si		
FG257			
FG258			
FG259			

* See page 49.

(continued)

TABLE VII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS (concluded)

Code*	Formula	Structure	User's notes
FG260	SiX		
FG261	SiX_2		
FG262	SiX_3		
FG263	Si_2		
FG264	Sn		
FG265	Te		
FG266			
FG267	Tl		
FG268	X		
FG269			
FG270	XE1		
FG271	Zn		

* See page 49.

Table VIII provides an index to the specific functional groups in terms of the names of the classes of compounds they represent. The chemist will appreciate that the intricacies of nomenclature are such as to prohibit the inclusion of all names which connote each individual group. Also, there are some functional groups which are not represented by unique compound class names, and thus do not appear in the index. Both systematic and trivial types of names are entered and the generous incorporation of secondary entries, with accompanying cross-references, further enhances utility.

The assignment of functional group keys solely on the basis of nomenclature ranges from hazardous to impossible. For those who wish to use it, the nomenclature index provides quick identification of the key(s) germane to a compound class. Applicability to a given structural query must be determined through examination of the structure of the functional group(s) as portrayed in Table VII.

Especial attention is directed to the manner in which the following classes of compounds are entered:

1. Esters, halides, and the thio- and seleno- analogues of systematically named acids are indexed as subentries under the class name of the acid. (All thio- acids, regardless of the number of O atoms which are replaced by S atoms, are referred to under a single subentry for the class. Example: Carboxylic acids, thio-.)

2. All keys in which a given element is displayed with a positive charge are indexed under the single entry of the form 'Element' cation, organo-, where 'Element' is the name of the element which carries the charge.

3. Keys which tag unequivocal carbon-metal bonds are indexed under 'Metal' compounds, organo-. where 'Metal' is the name of the individual metal involved.

4. Since all halogen-containing keys employ the general halogen symbol, X, these keys are indexed under generic names only. Example: Iodoso compounds are indexed as Haloso compounds.

TABLE VIII. SPECIFIC FUNCTIONAL GROUPS - NOMENCLATURE INDEX

Telluroxides, FG196
Thallium compounds, organo-, FG267
Thio acids, see Parent acid, thio-
Thio amides, see Parent amide, thio-
Thioaldehydes, see Aldehydes, thio-
Thioethers, see Sulfides
Thioketones, see Ketones, thio-
Thiols, FG245
Thiones, see Ketones, thio-
Thiosemicarbazide, see Semicarbazide, thio-
Thiosemicarbazone, see Semicarbazone, thio-
Thiourea derivatives, see Urea, thio-
Tin compounds, organo-, FG264
Triazene derivatives, org., see Diazoamino compounds

Urea derivs., FG67
see also Pseudourea derivs.
thio-, FG72
Ureides, see Urea derivs.
Urethans, see Carbamic acid esters

Vinyl alcohols, FG127-FG128

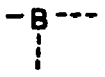
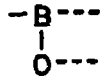
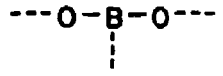
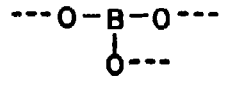
Xanthates, see Carbonic acid esters, thio-

"Ylium" compounds, Indexed under element carrying the charge.

Zinc compounds, organo-, FG271

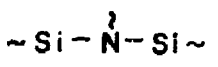
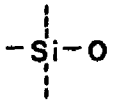
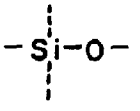
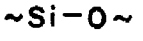
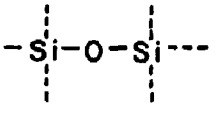
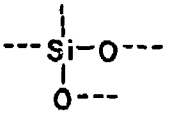
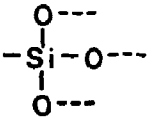
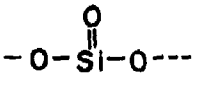
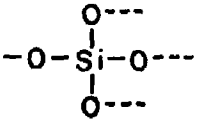
Tables IX through XXII present the same specific functional groups displayed in Table VII with the functional groups subdivided on the basis of the heteroelement(s) they contain. An additional table of those keys which contain carbon only is also provided. The ordering of the groups in each table is by Hill formula. In the case of a fragment which contains more than one heteroelement, the fragment is included in the table devoted to each of the respective heteroelements. Because of the prevalence of oxygen in the fragments, an exception to this multiple listing must be made with respect to this heteroelement (See Table XV).

TABLE IX. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING BORON

Code*	Formula	Structure	User's notes
FG18	B		
FG19	BO		
FG20	BO_2		
FG21			
FG22	BO_3		

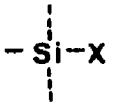
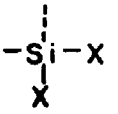
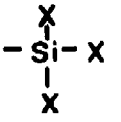
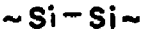
* See page 49.

TABLE X. SPECIFIC FUNCTIONAL GROUP (FG' CONTAINING SILICON

Code*	Formula	Structure	User's notes
FG166	NSi_2		
FG192	OSi		
FG193			
FG194			
FG195	OSi_2		
FG213	O_2Si		
FG227	O_3Si		
FG228			
FG233	O_4Si		
FG256	Si		

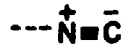
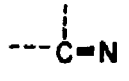
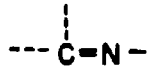
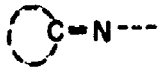
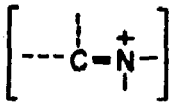
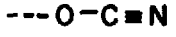
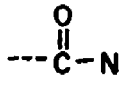
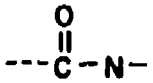
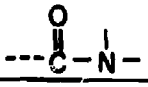
* See page 49. (continued)

TABLE X. SPECIFIC FUNCTIONAL GROUP (FG) CONTAINING SILICON (concluded)

Code*	Formula	Structure	User's notes
FG257			
FG258			
FG259			
FG260	SiX		
FG261	SiX_2		
FG262	SiX_3		
FG263	Si_2		

* See page 49.

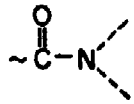
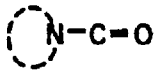
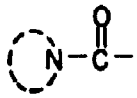
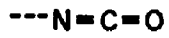
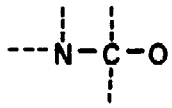
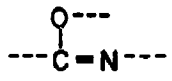
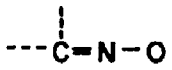
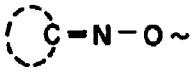
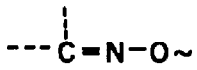
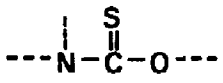
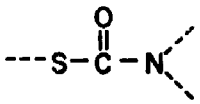
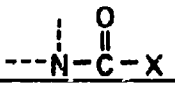
TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN

Code*	Formula	Structure	User's notes
FG24	CN		
FG25			
FG26			
FG27			
FG28			
FG29			
FG30			
FG31			
FG32			
FG33	CNO		
FG34			
FG35			
FG36			

* See page 49.

(continued)

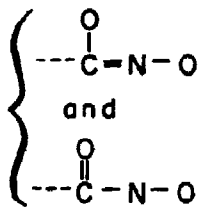
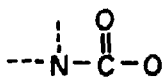
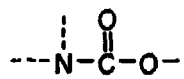
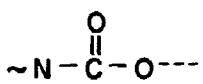
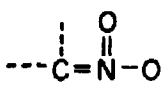
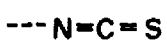
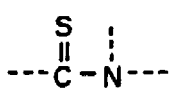
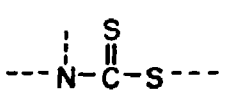
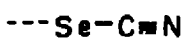
TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG37	CNO		
FG38			
FG39			
FG40			
FG41			
FG42			
FG43			
FG44			
FG45			
FG46	CNOS		
FG47			
FG48	CNOX		

* See page 49.

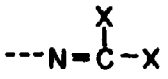
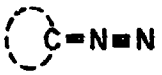
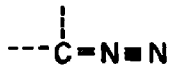
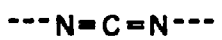
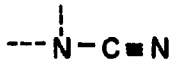
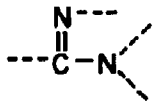
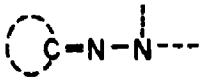
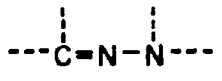
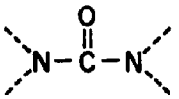
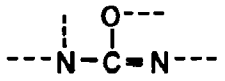
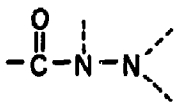
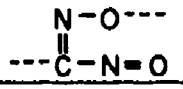
(continued)

TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG49	CNO_2		
FG50			
FG51			
FG52			
FG53			
FG54	CNS		
FG55			
FG56			
FG57	CNS_2		
FG58	CNSe		

* See page 49. (continued)

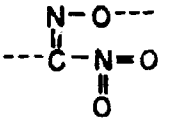
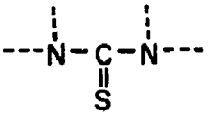
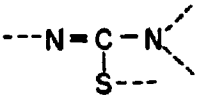
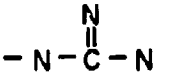
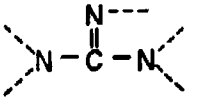
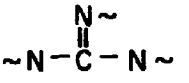
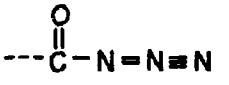
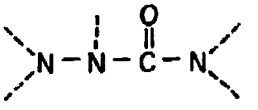
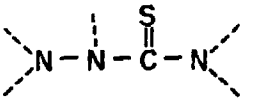
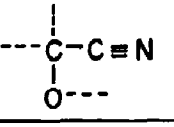
TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG59	CNX_2		
FG60	CN_2		
FG61			
FG62			
FG63			
FG64			
FG65			
FG66			
FG67	CN_2O		
FG68			
FG69			
FG70	CN_2O_2		

* See page 49.

(continued)

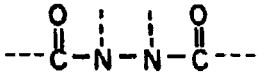
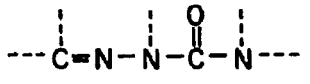
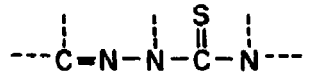
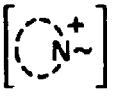
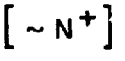
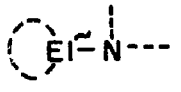
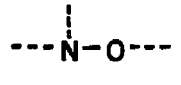
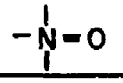
TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG71	CN_2O_3		
FG72	CN_2S		
FG73			
FG74	CN_3		
FG75			
FG76			
FG77	CN_3O		
FG78			
FG79	CN_3S		
FG123	C_2NO		

* See page 49.

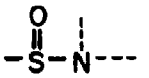
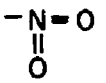
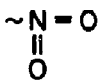
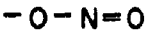
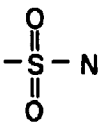
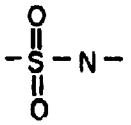
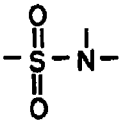
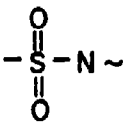
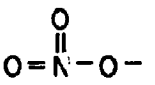
(continued)

TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG124	$C_2N_2O_2$		
FG125	C_2N_3O		
FG126	C_2N_3S		
FG143	N		
FG144			
FG145			
FG146			
FG147			
FG148	NEl		
FG149	NO		
FG150			
FG151			
FG152			

* See page 49. (continued)

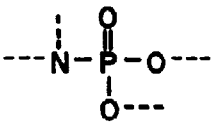
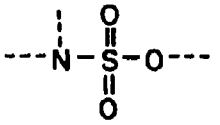
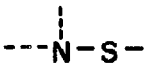
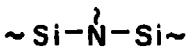
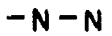
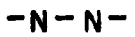
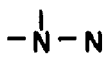
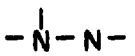
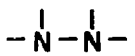
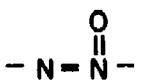
TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG153	NOS		
FG154	NO_2		
FG155			
FG156			
FG157	NO_2S		
FG158			
FG159			
FG160			
FG161	NO_3		

* See page 49

(continued)

TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (continued)

Code*	Formula	Structure	User's notes
FG162	NO_3P		
FG163	NO_3S		
FG164	NP		
FG165	NS		
FG166	NSi_2		
FG167	N_2		
FG168			
FG169			
FG170			
FG171			
FG172			
FG173			
FG174	N_2O		

* See page 49.

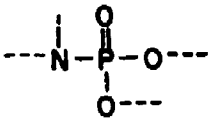
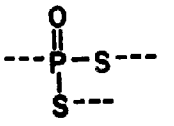
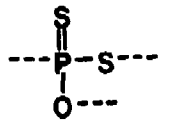
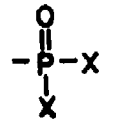
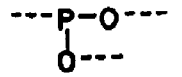
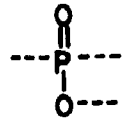
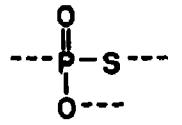
(continued)

TABLE XI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING NITROGEN (concluded)

Code*	Formula	Structure	User's notes
FG175	N_3	−N=N≡N	
FG176		~N=N−N~	

* See page 49.

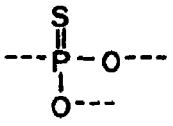
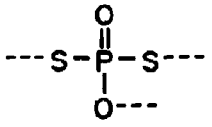
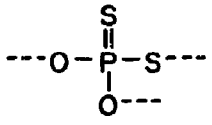
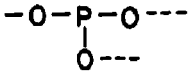
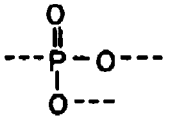
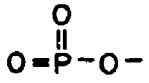
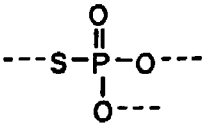
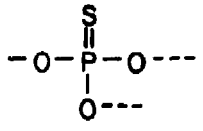
TABLE XII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING PHOSPHORUS

Code*	Formula	Structure	User's notes
FG162	NO_3P		
FG164	NP		
FG182	OP		
FG183	OPS_2		
FG184			
FG185	OPX_2		
FG200	O_2P		
FG201			
FG202	O_2PS		

* See page 49.

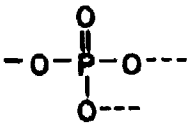
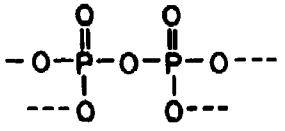
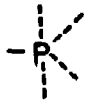
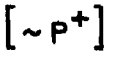
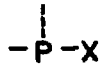
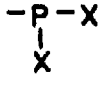
(continued)

TABLE XII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING PHOSPHORUS (continued)

Code*	Formula	Structure	User's notes
FG203			
FG204	O_2PS_2		
FG205			
FG217	O_3P		
FG218			
FG219			
FG220	O_3PS		
FG221	O_3PS		

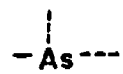
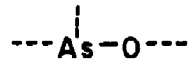
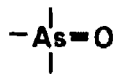
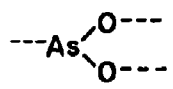
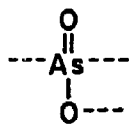
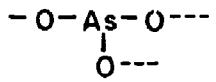
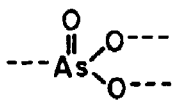
* See page 49. (continued)

TABLE XII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING PHOSPHORUS (concluded)

Code*	Formula	Structure	User's notes
FG231	O_4P		
FG235	O_7P_2		
FG236	P		
FG237			
FG238			
FG239			
FG240			
FG241	PX		
FG242	PX_2		
FG243	P_2		

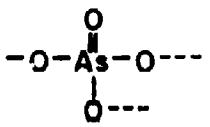
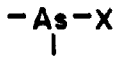
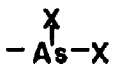
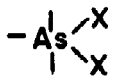
* See page 49.

TABLE XIII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING ARSENIC

Code*	Formula	Structure	User's notes
FG3	As		
FG4			
FG5	AsO		
FG6			
FG7			
FG8	AsO_2		
FG9			
FG10			
FG11	AsO_3		
FG12			

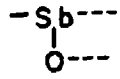
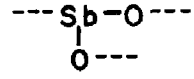
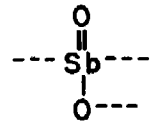
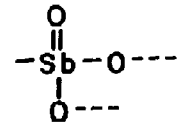
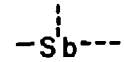
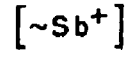
* See page 49. (continued)

TABLE XIII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING ARSENIC (concluded)

Code*	Formula	Structure	User's notes
FG13	AsO_4		
FG14	AsX		
FG15	AsX_2		
FG16			
FG17	As_2		

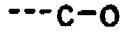
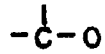
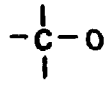
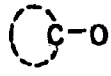
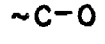
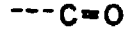
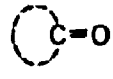
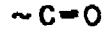
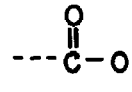
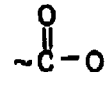
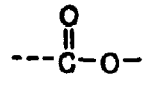
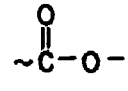
* See page 49.

TABLE XIV. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING ANTIMONY

Code*	Formula	Structure	User's notes
FG189	OSb		
FG190			
FG210	O_2Sb		
FG211			
FG226	O_3Sb		
FG252	Sb		
FG253			

* See page 49.

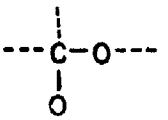
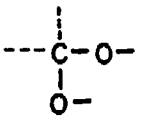
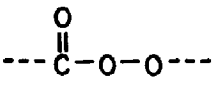
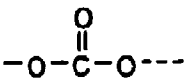
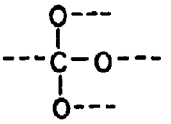
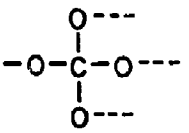
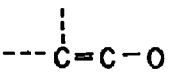
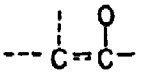
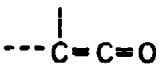
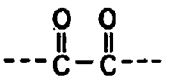
TABLE XV. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING OXYGEN AS THE ONLY HETEROELEMENT

Code*	Formula	Structure	User's notes
FG80	CO		
FG81			
FG82			
FG83			Note that keys containing both oxygen and one or more other heteroelements are listed only in the table(s) devoted to the other heteroelement(s).
FG84			
FG85			
FG86			
FG87			
FG88			
FG94	CO_2		
FG95			
FG96	CO_2		
FG97			

* See page 49.

(continued)

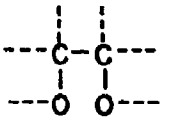
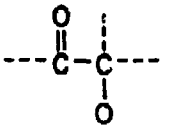
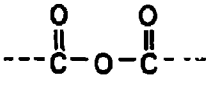
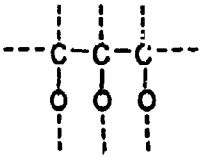
TABLE XV. SPECIFIC FUNCTIONAL GROUP (FG) KEYS
CONTAINING OXYGEN AS THE ONLY HETEROELEMENT (continued)

Code*	Formula	Structure	User's notes
FG98			
FG99			
FG102	CO_3		
FG103			
FG104			
FG105	CO_4		
FG127	C_2O		
FG128			
FG129	C_2O		
FG130	C_2O_2		

* See page 49.

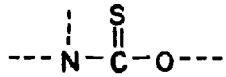
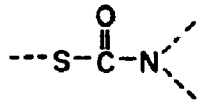
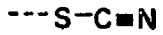
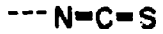
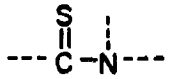
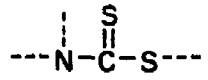
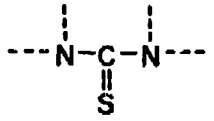
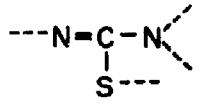
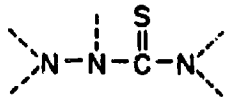
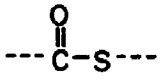
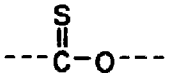
(continued)

TABLE XV. SPECIFIC FUNCTIONAL GROUP (FG) KEYS
CONTAINING OXYGEN AS THE ONLY HETEROELEMENT (concluded)

Code*	Formula	Structure	User's notes
FG131	C_2O_2		
FG132			
FG133	C_2O_3		
FG135	C_3O_3		
FG178	O	-O-	
FG179		$[\sim O^+]$	
FG199	O_2	-O-O---	

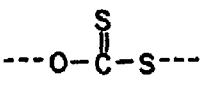
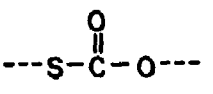
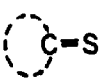
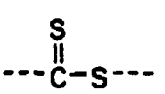
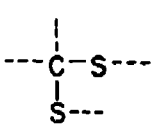
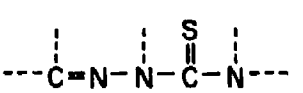
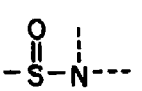
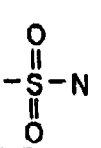
* See page 49.

TABLE XVI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SULFUR

Code*	Formula	Structure	User's notes
FG46	CNOS		
FG47	CNOS		
FG54	CNS		
FG55			
FG56			
FG57	CNS_2		
FG72	CN_2S		
FG73			
FG79	CN_3S		
FG89	COS		
FG90			

* See page 49. (continued)

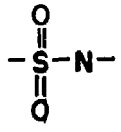
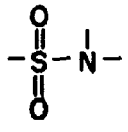
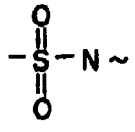
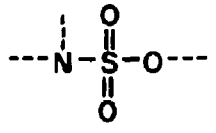
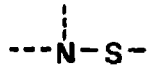
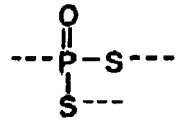
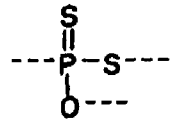
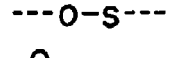
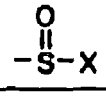
TABLE XVI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SULFUR (continued)

Code*	Formula	Structure	User's notes
FG91	COS_2		
FG100	CO_2S		
FG106	CS		
FG107			
FG108			
FG109			
FG110	CS_2		
FG111			
FG126	C_2N_3S		
FG153	NOS		
FG157	NO_2S		

(continued)

* See page 49.

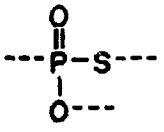
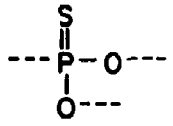
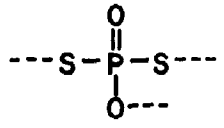
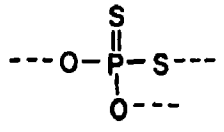
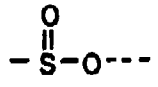
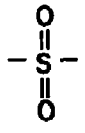
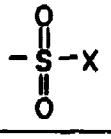
TABLE XVI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SULFUR (continued)

Code*	Formula	Structure	User's notes
FG158			
FG159	NO_2S		
FG160			
FG163	NO_3S		
FG165	NS		
FG183	OPS_2		
FG184			
FG186	OS		
FG187			
FG188	OSX		

* See page 49.

(continued)

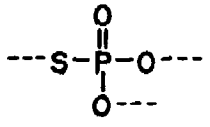
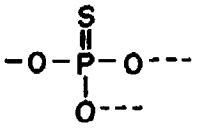
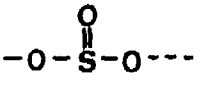
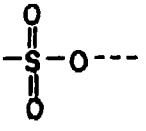
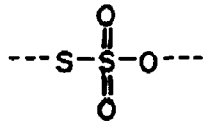
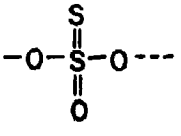
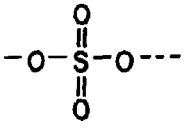
TABLE XVI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SULFUR (continued)

Code*	Formula	Structure	User's notes
FG202	O_2PS		
FG203			
FG204	O_2PS_2		
FG205			
FG206	O_2S		
FG207			
FG208			
FG209	O_2SX		

* See page 49.

(continued)

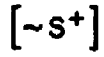
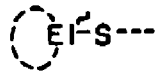
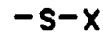
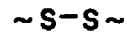
TABLE XVI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SULFUR (continued)

Code*	Formula	Structure	User's Notes
FG220	O_3PS		
FG221			
FG222	O_3S		
FG223			
FG224	O_3S_2		
FG225			
FG232	O_4S		
FG245	S		
FG246			

* See page 49.

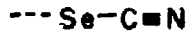
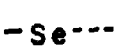
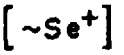
(continued)

TABLE XVI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SULFUR (concluded)

Code*	Formula	Structure	User's notes
FG247	S		
FG248	SE1		
FG249			
FG250	SX		
FG251	S_2		

* See page 49.

TABLE XVII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING SELENIUM

Code*	Formula	Structure	User's notes
FG58	CNSe		
FG191	OSe		
FG212	O_2Se		
FG254	Se		
FG255			

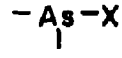
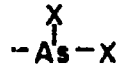
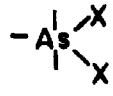
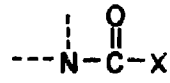
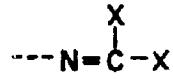
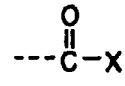
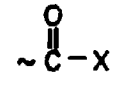
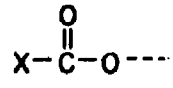
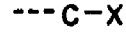
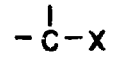
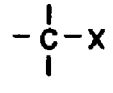
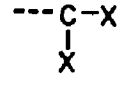
* See page 49.

TABLE XVIII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING TELLURIUM

Code*	Formula	Structure	User's notes
FG196	OTe	~Te=O	
FG214	O_2Te		
FG265	Te	-Te---	
FG266		[~Te+]	

* See page 49.

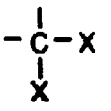
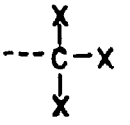
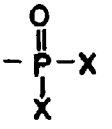
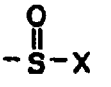
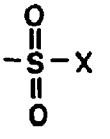
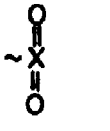
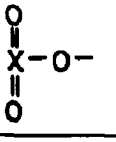
TABLE XIX. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING HALOGENS

Code*	Formula	Structure	User's notes
FG14	AsX		
FG15	AsX_2		
FG16			
FG48	CNOX		
FG59	CNX_2		
FG92	COX		
FG93			
FG101	CO_2X		
FG112	CX		
FG113			
FG114			
FG115	CX_2		

(continued)

* See page 49.

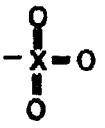
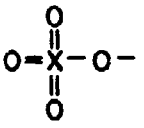
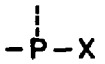
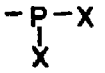
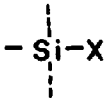
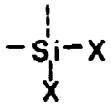
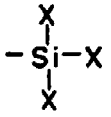
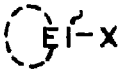
TABLE XIX. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING HALOGENS (continued)

Code*	Formula	Structure	User's notes
FG116			
FG117	CX_3		
FG185	OPX_2		
FG188	OSX		
FG197	OX		
FG198			
FG209	O_2SX		
FG215	O_2X		
FG216	O_2X		
FG229	O_3X		

(continued)

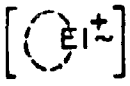
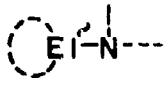
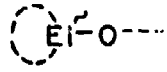
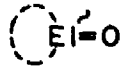
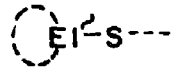
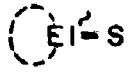
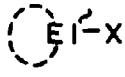
* See page 49.

TABLE XIX. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING HALOGENS (concluded)

Code*	Formula	Structure	User's notes
FG230			
FG234	O_4X		
FG241	PX		
FG242	PX_2		
FG250	SX		
FG260	SiX		
FG261	SiX_2		
FG262	SiX_3		
FG268	X		
FG269			
FG270	XE1		

* See page 49.

TABLE XX. SPECIFIC FUNCTIONAL GROUP (FG) KEYS
CONTAINING AN UNSPECIFIED HETEROATOM

Code*	Formula	Structure	User's notes
FG23	CE1		Caution! See explanatory note 1, p. 46.
FG121	C_2E1		Caution! See explanatory note 1, p. 46.
FG122	C_2E1_2		Caution! See explanatory note 1, p. 46.
FG137	E1		
FG148	NE1		
FG180	CE1		
FG181			
FG248	SE1		
FG249			
FG270	XE1		

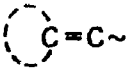
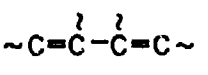
* See page 49.

TABLE XXI. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING A C-METAL BOND

Code*	Formula	Structure	User's Notes
FG1	Ag	−Ag	
FG2	Al	−Al~	
FG138	Fe	−Fe~	
FG139	Hg	−Hg~	
FG140	K	−K	
FG141	Li	−Li	
FG142	Mg	−Mg~	
FG177	Na	−Na	
FG244	Pb	−Pb~	
FG264	Sn	−Sn~	
FG267	Tl	−Tl~	
FG271	Zn	−Zn~	

* See page 49.

TABLE XXII. SPECIFIC FUNCTIONAL GROUP (FG) KEYS CONTAINING CARBON ONLY

Code*	Formula	Structure	User's notes
FG118	C_2	---C≡C---	
FG119			
FG120	C_2	~C≡C~	
FG134	C_3	~C≡C≡C~	
FG136	C_4		

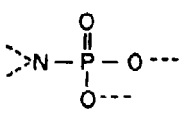
* See page 49.

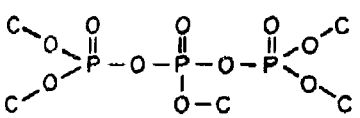
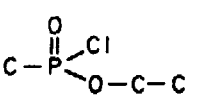
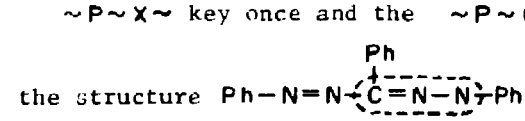
2.2.8 Nonspecific Diatomic Functional Group (NC) Keys

In addition to the specific functional group keys described in Section 2.2.7, CIDS utilizes two families of nonspecific functional group keys. The family presented in this section embraces all possible diatomic keys involving those heteroelements which occur generously in organic combination. These include the elements B, Si, N, P, As, Sb, O, S, Se, Te, and X, where X represents F, Cl, Br, and I.

It will be observed that each of these keys stipulates only that the two heteroatoms are bonded together; the bond may be single or multiple and it matters not what other atoms or groups of atoms are attached to the two heteroatoms.

Three additional features are noted:

(1) These keys are assigned only if the functional group represented is NOT included in the specific keys of Section 2.2.7. Thus, for example, the phosphoramidic acids and esters are represented in Section 2.2.7 by the fragment  and thus neither the ~N~P~ nor the ~P~O~ key would be assigned to any one of these acids or esters.

(2) Overlap (Section 2.2.7) is frequently observed with these keys. Thus, for example, the ~P~O~ key is assigned 12 times to the structure  and the structure  receives the ~P~X~ key once and the ~P~O~ key twice. The encircled portion of the structure  provides an example of an ND key (~N~N~) overlapping a specific functional group key (~C=N~).

(3) As with the specific functional group keys (Note 11, page 48), the letter R is appended to the code in instances in which either or both of the hanging bonds represents direct attachment to a ring.

Table XXIII lists the nonspecific diatomic keys by Hill Formula ordering and Table XXIV charts them conveniently by key number.

TABLE XXIII. NONSPECIFIC DIATOMIC FUNCTIONAL GROUP (ND) KEYS

(Hill ordered)

Formula	Code*	Structure	User's notes
AsB	ND1	~As~B~	
AsN	ND2	~As~N~	
AsO	ND3	~As~O~	
AsP	ND4	~As~P~	
AsS	ND5	~As~S~	
AsSb	ND6	~As~Sb~	
AsSe	ND7	~As~Se~	
AsSi	ND8	~As~Si~	
AsTe	ND9	~As~Te~	
AsX	ND10	~As~X~	
As_2	ND11	~As~As~	
BN	ND12	~B~N~	
BO	ND13	~B~O~	
BP	ND14	~B~P~	
BS	ND15	~B~S~	
BSb	ND16	~B~Sb~	
BSe	ND17	~B~Se~	
BSi	ND18	~B~Si~	
BTe	ND19	~B~Te~	
BX	ND20	~B~X~	
B_2	ND21	~B~B~	
NO	ND22	~N~O~	
NP	ND23	~N~P~	

* The letter R is appended to the code whenever one or both of the hanging bonds represents direct attachment to a ring.

(continued)

TABLE XXIII. NONSPECIFIC DIATOMIC FUNCTIONAL GROUP (ND) KEYS (continued)
(Hill ordered)

Formula	Code*	Structure	User's notes
NS	ND24	~N~S~	
NSb	ND25	~N~Sb~	
NSe	ND26	~N~Se~	
NSi	ND27	~N~Si~	
NTe	ND28	~N~Te~	
NX	ND29	~N~X~	
N_2	ND30	~N~N~	
OP	ND31	~O~P~	
OS	ND32	~O~S~	
OSb	ND33	~O~Sb~	
OSe	ND34	~O~Se~	
OSi	ND35	~O~Si~	
OTe	ND36	~O~Te~	
OX	ND37	~O~X~	
O_2	ND38	~O~O~	
PS	ND39	~P~S~	
PSb	ND40	~P~Sb~	
PSe	ND41	~P~Se~	
PSi	ND42	~P~Si~	
PTe	ND43	~P~Te~	
PX	ND44	~P~X~	
P_2	ND45	~P~P~	
SSb	ND46	~S~Sb~	

* See page 120.

(continued)

TABLE XXIII. NONSPECIFIC DIATOMIC FUNCTIONAL GROUP (ND) KEYS (concluded)
(Hill ordered)

Formula	Code*	Structure	User's notes
SSe	ND47	~S~Se~	
SSi	ND48	~S~Si~	
STe	ND49	~S~Te~	
SX	ND50	~S~X~	
S_2	ND51	~S~S~	
SbSe	ND52	~Sb~Se~	
SbSi	ND53	~Sb~Si~	
SbTe	ND54	~Sb~Te~	
SbX	ND55	~Sb~X~	
Sb_2	ND56	~Sb~Sb~	
SeSi	ND57	~Se~Si~	
SeTe	ND58	~Se~Te~	
SeX	ND59	~Se~X~	
Se_2	ND60	~Se~Se~	
SiTe	ND61	~Si~Te~	
SiX	ND62	~Si~X~	
Si_2	ND63	~Si~Si~	
TeX	ND64	~Te~X~	
Te_2	ND65	~Te~Te~	
X_2	ND66	~X~X~	

* See page 120.

TABLE XXIV. SCHEMA OF NONSPECIFIC DIATOMIC FUNCTIONAL GROUP (ND) KEYS*

	As	B	N	O	P	S	Sb	Se	Si	Te	X
As	ND11	ND1	ND2	ND3	ND4	ND5	ND6	ND7	ND8	ND9	ND10
B		ND21	ND12	ND13	ND14	ND15	ND16	ND17	ND18	ND19	ND20
N			ND30	ND22	ND23	ND24	ND25	ND26	ND27	ND28	ND29
O				ND38	ND31	ND32	ND33	ND34	ND35	ND36	ND37
P					ND45	ND39	ND40	ND41	ND42	ND43	ND44
S						ND51	ND46	ND47	ND48	ND49	ND50
Sb							ND56	ND52	ND53	ND54	ND55
Se								ND60	ND57	ND58	ND59
Si									ND63	ND61	ND62
Te										ND65	ND64
X											ND66

* See page 120.

2.2.9 Nonspecific Monatomic Functional Group (NM) Keys

The nonspecific monatomic functional group keys comprise the least specific family of functional group keys in the system. As readily apparent from the structure, each key merely specifies the presence of a heteroatom in the structure in an environment different from that in any of the keys in Sections 2.2.7 and 2.2.8. In effect, these keys provide a guarantee that no compound containing a functional group will "get lost", i.e., will escape having assigned to it a functional group key.

The system is designed to minimize the need for these keys in the processing of queries. Consonant with this aim, it is visualized that printouts of all compounds to which one of these keys has been assigned will be examined periodically to see if a particular functional group is occurring with sufficient frequency to warrant the inclusion of a specific key for it.

The individual keys of this family are ordered alphabetically in Table XXV. The three rules which govern their assignment are:

(1) They are assigned only in the absence of a more specific key representing the functional group involved;

(2) If the functional group involved contains more than one heteroelement, the structure is assigned the key appropriate to each heteroelement.

(3) The letter R is appended to the code in instances in which the hanging bond represents direct attachment to a ring.

TABLE XXV. NONSPECIFIC MONATOMIC FUNCTIONAL GROUP (NM) KEYS

(alphabetical order)

Formula	Code*	Structure	User's notes
As	NM1	~ As	
B	NM2	~ B	
N	NM3	~ N	
O	NM4	~ O	
P	NM5	~ P	
S	NM6	~ S	
Sb	NM7	~ Sb	
Se	NM8	~ Se	
Si	NM9	~ Si	
Te	NM10	~ Te	
X	NM11	~ X	

* The letter R is appended to the code in instances in which the hanging bond represents direct attachment to a ring.

2.2.10 Hydrocarbon Radical (HR) Keys

The employment of generic and specific cyclic nuclei keys renders it unnecessary to employ cyclic hydrocarbon radicals (HR) as keys. The system thus includes only acyclic HR keys and, furthermore, the selection of these (as with the specific functional group keys) is restricted on the basis of expected frequency of occurrence and conjectured utility in processing queries. The system inventory of hydrocarbon radicals consists of 61 specific radicals and 15 generic radicals, and a scheme showing the distribution of these 76 radicals among the various types is provided in Table XXVI. Distinguishment in terms of attachment of each radical to heteroatom(s) and to ring(s) leads to the 181 hydrocarbon radical keys of the system.

The multiple assignment characteristics of HR keys is worthy of special note. For example, a structure which contains a methyl group attached to a ring heteroatom is assigned both the HR1E (methyl to heteroatom) and the HR1R (methyl to ring) keys. Similarly, the generic radical, HRG29E, is assigned to any structure containing a C_5H_{11} radical attached to a heteroatom, including those in which the radical is any one of the specific C_5H_{11} radicals in the system, viz., HR25E, HR26E, HR27E, or HR28E.

Table XXVII, page 128, presents a complete listing of CIDS hydrocarbon radicals ordered in Hill formula fashion with the symbols El (any ring or non-ring heteroatom) and R (any ring atom) participating in the alphabetization. Shown also are the CIDS code and the structure of each radical. With regard to the structure, especial attention is called to the use of the notation $(C)_n$ to mean a string of n methylene, $-CH_2-$, groups, and the notation C_n to mean a saturated hydrocarbon radical having n C atoms in any structural configuration. In either case, n is sometimes one specified number, e.g., $(C)_5$ and C_5, and at other times covers a specified range.

Table XXVIII, page 138 , provides the reverse kind of an index, i.e., the ordering is by CIDS code and the reference is to the Hill formula. The structures are not repeated since they are readily available from the preceding table.

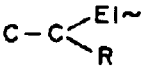
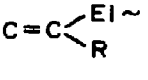
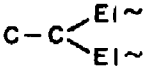
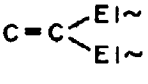
Table XXIX, page 142, provides a nomenclature approach to the CIDS hydrocarbon radicals. It will be recalled, however, that the radical name often does not appear in the name of the compound containing it. Thus, for example, the name 2-methyl-2-propanol does not identify the presence of the tert-butyl radical; the name ethanolamine renders cryptic the ethylene radical; etc.

TABLE XXVI. SCHEMA OF CIDS HYDROCARBON RADICAL KEYS

Number of Carbon Atoms	Hydrocarbon Radicals						
	Saturated						Unsaturated
	Monovalent				Polyvalent		
	Normal	Iso-form	Others (Specific)	Generic*	Polymeth-ylenes	Others (Specific)	
1	√				√		
2	√				√	1	4
3	√	√			√	4	3
4	√	√	2		√		
5	√	√	2	√	√		
6	√	√		√	√		
7	√	√		√	√		
8	√	√	1	√	√		
9	√			√	√		
10	√			√	√		
11	√			√	√		
12	√			√	√		
13	√			√	√		
14	√			√	√		
15	√			√	√		
16	√			√	√		
17	√			√	√		
18	√			√	√		
> 18	√			√	√		

* Any configuration of C atoms.

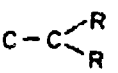
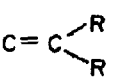
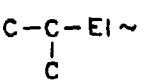
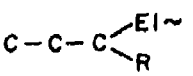
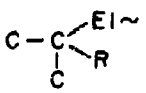
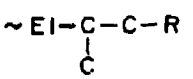
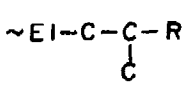
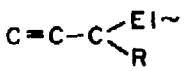
TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS

Formula*	Code	Structure	User's notes
CEl	HR1E	C–El~	
CElR	HR2ER	~El–C–R	
CEl_2	HR2EE	~El–C–El~	
CR	HR1R	C–R	
CR_2	HR2RR	R–C–R	
C_2El	HR3E	C–C–El~	
	HR4E	C=C–El~	
	HR5E	C≡C–El~	
C_2ElR	HR6ER	~El–C–C–R	
	HR7ER		
	HR8ER	~El–C=C–R	
	HR9ER		
C_2El_2	HR6EE	~El–C–C–El~	
	HR7EE		
	HR8EE	~El–C=C–El~	
	HR9EE		
C_2R	HR3R	C–C–R	

* Ordered in Hill style formulas showing number of C atoms in radical and number of attachments to heteroatoms (El) and/or ring atoms(R).

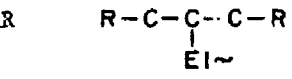
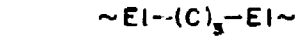
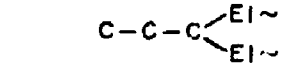
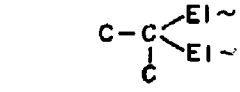
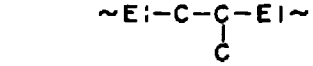
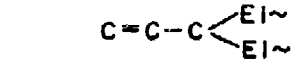
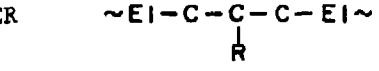
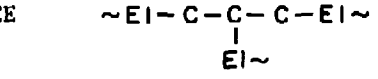
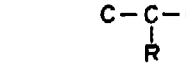
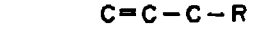
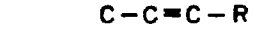
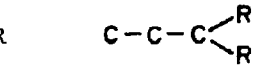
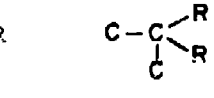
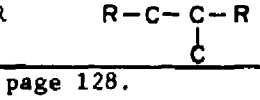
(continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
C_2R	HR4R	C=C-R	
	HR5R	C≡C-R	
C_2R_2	HR6RR	R-C-C-R	
	HR7RR		
	HR8RR	R-C=C-R	
	HR9RR		
C_3El	HR10E	C-C-C-El~	
	HR11E		
	HR12E	C=C-C-El~	
	HR13E	C-C=C-El~	
C_3ElR	HR14ER	~El-$(C)_3$-R	
	HR15ER		
	HR16ER		
	HR17ER1		
	HR17ER2		
	HR18ER		

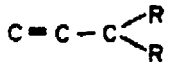
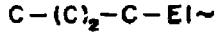
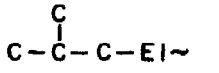
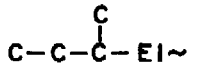
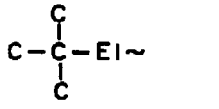
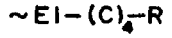
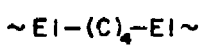
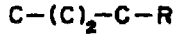
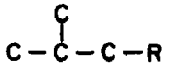
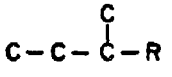
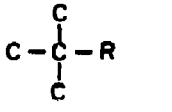
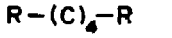
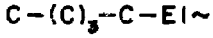
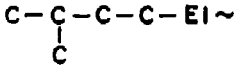
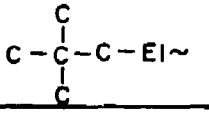
* See footnote, page 128. (continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
$C_3El R_2$	HR19ERR		
C_3El_2	HR14EE		
	HR15EE		
	HR16EE		
	HR17EE		
	HR18EE		
C_3El_2R	HR19EER		
C_3El_3	HR19EEE		
C_3R	HR10R		
	HR11R		
	HR12R		
	HR13R		
C_3R_2	HR14RR		
	HR15RR		
	HR16RR		
	HR17RR		

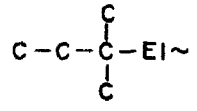
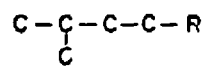
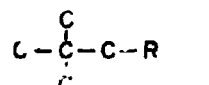
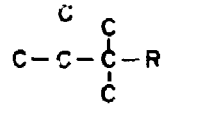
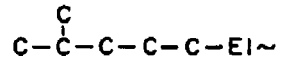
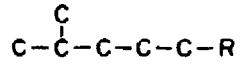
* See footnote, page 128. (continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
C_3R_2	HR18RR		
C_3R_3	HR19RRR		
C_4El	HR20E		
	HR21E		
	HR22E		
	HR23E		
C_4ElR	HR24ER		
C_4El_2	HR24EE		
C_4R	HR20R		
	HR21R		
	HR22R		
	HR23R		
C_4R_2	HR24RR		
C_5El	HR25E		
	HR26E		
	HR27E		

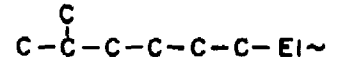
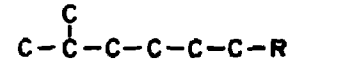
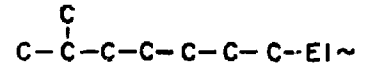
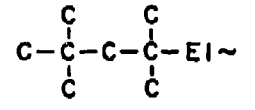
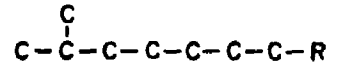
* See footnote, page 128. (continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
C_5El	HR28E		
	HR29E	$C_5-El\sim$	
C_5ElR	HR30ER	$\sim El-(C)_5-R$	
C_5El_2	HR30EE	$\sim El-(C)_5-El\sim$	
C_5R	HR25R	$C-(C)_3-C-R$	
	HR26R		
	HR27R		
	HR28R		
	HRG29R	C_5-R	
C_5R_2	HR30RR	$R-(C)_5-R$	
C_6El	HR31E	$C-(C)_4-C-El\sim$	
	HR32E		
	HRG33E	$C_6-El\sim$	
C_6ElR	HR34ER	$\sim El-(C)_6-R$	
C_6El_2	HR34EE	$\sim El-(C)_6-El\sim$	
C_6R	HR31R	$C-(C)_4-C-R$	
	HR32R		
	HRG33R	C_6-R	

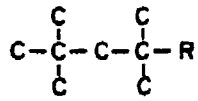
* See footnote, page 128. (continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
C_6R_2	HR34RR	R–(C)$_6$–R	
C_7El	HR35E	C–(C)$_5$–C–El~	
	HR36E		
	HRG37E	C_7–El~	
C_7ElR	HR38ER	~El–(C)$_7$–R	
C_7El_2	HR38EE	~El–(C)$_7$–El~	
C_7R	HR35R	C–(C)$_5$–C–R	
	HR36R		
	HRG37R	C_7–R	
C_7R_2	HR38RR	R–(C)$_7$–R	
C_8El	HR39E	C–(C)$_6$–C–El~	
	HR40E		
	HR41E		
	HRG42E	C_8–El~	
C_8ElR	HR43ER	~El–(C)$_8$–R	
C_8El_2	HR43EE	~El–(C)$_8$–El~	
C_8R	HR39R	C–(C)$_6$–C–R	
	HR40R		

* See footnote, page 128. (continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
C_8R	HR41R		
	HRG42R	C_8-R	
C_8R_2	HR43RR	$R-(C)_8-R$	
C_9El	HR44E	$C-(C_7)-C-El\sim$	
	HR45E	$C_9-El\sim$	
C_9ElR	HR46ER	$\sim El-(C)_9-R$	
C_9El_2	HR46EE	$\sim El-(C)_9-El\sim$	
C_9R	HR44R	$C-(C)_7-C-R$	
	HRG45R	C_9-R	
C_9R_2	HR46RR	$R-(C)_9-R$	
$C_{10}El$	HR47E	$C-(C)_8-C-El\sim$	
	HRG48E	$C_{10}-El\sim$	
$C_{10}ElR$	HR49ER	$\sim El-(C)_{10}-R$	
$C_{10}El_2$	HR49EE	$\sim El-(C)_{10}-El\sim$	
$C_{10}R$	HR47R	$C-(C)_8-C-R$	
	HRG48R	$C_{10}-R$	
$C_{10}R_2$	HR49RR	$R-(C)_{10}-R$	
$C_{11}El$	HR50E	$C-(C_9)-C-El\sim$	
	HRG51E	$C_{11}-El\sim$	
$C_{11}ElR$	HR52ER	$\sim El-(C)_{11}-R$	
$C_{11}El_2$	HR52EE	$\sim El-(C)_{11}-El\sim$	
$C_{11}R$	HR50R	$C-(C)_9-C-R$	

* See footnote, page 128.

(continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
$C_{11}R$	HRG51R	$C_{11}-R$	
$C_{11}R_2$	HR52Rk	$R-(C)_{11}-R$	
$C_{12}El$	HR53E	$C-(C)_{10}-C-El\sim$	
	HRG54E	$C_{12}-El\sim$	
$C_{12}ElR$	HR55ER	$\sim El-(C)_{12}-R$	
$C_{12}El_2$	HR55EE	$\sim El-(C)_{12}-El\sim$	
$C_{12}R$	HR53R	$C-(C)_{10}-C-R$	
	HRG54R	$C_{12}-R$	
$C_{12}R_2$	HR55RR	$R-(C)_{12}-R$	
$C_{13}El$	HR56E	$C-(C)_{11}-C-EL\sim$	
	HRG57E	$C_{13}-El\sim$	
$C_{13}ElR$	HR58ER	$\sim El-(C)_{13}-R$	
$C_{13}El_2$	HR58EE	$\sim El-(C)_{13}-El\sim$	
$C_{13}R$	HR56R	$C-(C)_{11}-C-R$	
	HRG57R	$C_{13}-R$	
$C_{13}R_2$	HR58RR	$R-(C)_{13}-R$	
$C_{14}El$	HR59E	$C-(C)_{12}-C-El\sim$	
	HRG60E	$C_{14}-El\sim$	
$C_{14}ElR$	HR61ER	$\sim El-(C)_{14}-R$	
$C_{14}El_2$	HR61EE	$\sim El-(C)_{14}-El\sim$	
$C_{14}R$	HR59R	$C-(C)_{12}-C-R$	
	HRG60R	$C_{14}-R$	

* See footnote, page 128.

(continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (continued)

Formula*	Code	Structure	User's notes
$C_{14}R_2$	HR61RR	R−(C)$_{14}$−R	
$C_{15}El$	HR62E	C−(C)$_{13}$−C−El~	
	HRG63E	C_{15}−El~	
$C_{15}ElR$	HR64ER	~El−(C)$_{15}$−R	
$C_{15}El_2$	HR64EE	~El−(C)$_{15}$−El~	
$C_{15}R$	HR62R	C−(C)$_{13}$−C−R	
	HRG63R	C_{15}−R	
$C_{15}R_2$	HR64RR	R−(C)$_{15}$−R	
$C_{16}El$	HR65E	C−(C)$_{14}$−C−El~	
	HRG66E	C_{16}−El~	
$C_{16}ElR$	HR67ER	~El−(C)$_{16}$−R	
$C_{16}El_2$	HR67EE	~El−(C)$_{16}$−El~	
$C_{16}R$	HR65R	C−(C)$_{14}$−C−R	
	HRG66R	C_{16}−R	
$C_{16}R_2$	HR67RR	R−(C)$_{16}$−R	
$C_{17}El$	HR68E	C−(C)$_{15}$−C−El~	
	HRG69E	C_{17}−El~	
$C_{17}ElR$	HR70ER	~El−(C)$_{17}$−R	
$C_{17}El_2$	HR70EE	~El−(C)$_{17}$−El~	
$C_{17}R$	HR68R	C−(C)$_{15}$−C−R	
	HRG69R	C_{17}−R	
$C_{17}R_2$	HR70RR	R−(C)$_{17}$−R	
$C_{18}El$	HR71E	C−(C)$_{16}$−C−El~	

* See footnote, page 128. (continued)

TABLE XXVII. CIDS HYDROCARBON RADICAL KEYS (concluded)

Formula*	Code	Structure	User's notes
$C_{18}El$	HRG72E	$C_{18}-El\sim$	
$C_{18}ElR$	HR73ER	$\sim El-(C)_{18}-R$	
$C_{18}El_2$	HR73EE	$\sim El-(C)_{18}-El\sim$	
$C_{18}R$	HR71R	$C-(C)_{16}-C-R$	
	HRG72R	$C_{18}-R$	
$C_{18}R_2$	HR73RR	$R-(C)_{18}-R$	
C_nEl (n>18)	HR74E	$C-(C)_n-C-El\sim$ (n>16)	
	HRG75E	$C_n-El\sim$ (n>18)	
C_nElR (n>18)	HR76ER	$\sim El-(C)_n-R$ (n>18)	
C_nEl_2 (n>18)	HR76EE	$\sim El-(C)_n-El\sim$ (n>18)	
C_nR (n>18)	HR74R	$C-(C)_n-C-R$ (n>16)	
	HRG75R	C_n-R (n>18)	
C_nR_2 (n>18)	HR76RR	$R-(C)_n-R$ (n>18)	

* See footnote, page 128.

TABLE XXVIII. CIDS CODE INDEX TO HYDROCARBON RADICAL KEYS

Code	Formula	Code	Formula
HR1E	CE1	HR11E	C_3E1
HR1R	CR	HR11R	C_3R
HR2EE	$CE1_2$	HR12E	C_3E1
HR2ER	CE1R	HR12R	C_3R
HR2RR	CR_2	HR13E	C_3E1
HR3E	C_2E1	HR13R	C_3R
HR3R	C_2R	HR14EE	C_3E1_2
HR4E	C_2E1	HR14ER	C_3E1R
HR4R	C_2R	HR14RR	C_3R_2
HR5E	C_2E1	HR15EE	C_3E1_2
HR5R	C_2R	HR15ER	C_3E1R
HR6EE	C_2E1_2	HR15RR	C_3R_2
HR6ER	C_2E1R	HR16EE	C_3E1_2
HR6RR	C_2R_2	HR16ER	C_3E1R
HR7EE	C_2E1_2	HR16RR	C_3R_2
HR7ER	C_2E1R	HR17EE	C_3E1_2
HR7RR	C_2R_2	HR17ER1	C_3E1R
HR8EE	C_2E1_2	HR17ER2	C_3E1R
HR8ER	C_2E1R	HR17RR	C_3R_2
HR8RR	C_2R_2	HR18EE	C_3E1_2
HR9EE	C_2E1_2	HR18ER	C_3E1R
HR9ER	C_2E1R	HR18RR	C_3R_2
HR9RR	C_2R_2	HR19EEE	C_3E1_3
HR10E	C_3E1	HR19EER	C_3E1_2R
HR10R	C_3R	HR19ERR	C_3E1R_2

(continued)

Code	Formula	Code	Formula
HR19RRR	C_3R_3	HR32R	C_6R
HR20E	C_4E1	HR34EE	C_6E1_2
HR20R	C_4R	HR34ER	C_6E1R
HR21E	C_4E1	HR34RR	C_6R_2
HR21R	C_4R	HR35E	C_7E1
HR22E	C_4E1	HR35R	C_7R
HR22R	C_4R	HR36E	C_7E1
HR23E	C_4E1	HR36R	C_7R
HR23R	C_4R	HR38EE	C_7E1_2
HR24EE	C_4E1_2	HR38ER	C_7E1R
HR24ER	C_4E1R	HR38RR	C_7R_2
HR24RR	C_4R_2	HR39E	C_8E1
HR25E	C_5E1	HR39R	C_8R
HR25R	C_5R	HR40E	C_8E1
HR26E	C_5E1	HR40R	C_8R
HR26R	C_5R	HR41E	C_8E1
HR27E	C_5E1	HR41R	C_8R
HR27R	C_5R	HR43EE	C_8E1_2
HR28E	C_5E1	HR43ER	C_8E1R
HR28R	C_5R	HR43RR	C_8R_2
HR30EE	C_5E1_2	HR44E	C_9E1
HR30ER	C_5E1R	HR44R	C_9R
HR30RR	C_5R_2	HR46EE	C_9E1_2
HR31E	C_6E1	HR46ER	C_9E1R
HR31R	C_6R	HR46RR	C_9R_2
HR32E	C_6E1	HR47E	$C_{10}E1$

(continued)

Code	Formula	Code	Formula
HR47R	$C_{10}R$	HR64ER	$C_{15}E1R$
HR49EE	$C_{10}E1_2$	HR64RR	$C_{15}R_2$
HR49ER	$C_{10}E1R$	HR65E	$C_{16}E1$
HR49RR	$C_{10}R_2$	HR65R	$C_{16}R$
HR50E	$C_{11}E1$	HR67EE	$C_{16}E1_2$
HR50R	$C_{11}R$	HR67ER	$C_{16}E1R$
HR52EE	$C_{11}E1_2$	HR67RR	$C_{16}R_2$
HR52ER	$C_{11}E1R$	HR68E	$C_{17}E1$
HR52RR	$C_{11}R_2$	HR68R	$C_{17}R$
HR53E	$C_{12}E1$	HR70EE	$C_{17}E1_2$
HR53R	$C_{12}R$	HR70ER	$C_{17}E1R$
HR55EE	$C_{12}E1_2$	HR70RR	$C_{17}R_2$
HR55ER	$C_{12}E1R$	HR71E	$C_{18}E1$
HR55RR	$C_{12}R_2$	HR71R	$C_{18}R$
HR56E	$C_{13}E1$	HR73EE	$C_{18}E1_2$
HR56R	$C_{13}R$	HR73ER	$C_{18}E1R$
HR58EE	$C_{13}E1_2$	HR73RR	$C_{18}R_2$
HR58ER	$C_{13}E1R$	HR74E	C_nE1 (n>18)
HR58RR	$C_{13}R_2$	HR74R	C_nR (n>18)
HR59E	$C_{14}E1$	HR76EE	C_nE1_2 (n>18)
HR59R	$C_{14}R$	HR76ER	C_nE1R (n>18)
HR61EE	$C_{14}E1R_2$	HR76RR	C_nR_2 (n>18)
HR61ER	$C_{14}E1R$	HRG29E	C_5E1
HR61RR	$C_{14}R_2$	HRG29R	C_5R
HR62E	$C_{15}E1$	HRG33E	C_6E1
HR62R	$C_{15}R$	HRG33R	C_6R
HR64EE	$C_{15}E1_2$	HRG37E	C_7E1

(continued)

Code	Formula
HRG37R	C_7R
HRG42E	C_8E1
HRG42R	C_8R
HRG45E	C_9E1
HRG45R	C_9R
HRG48E	$C_{10}E1$
HRG48R	$C_{10}R$
HRG51E	$C_{11}E1$
HRG51R	$C_{11}R$
HRG54E	$C_{12}E1$
HRG54R	$C_{12}R$
HRG57E	$C_{13}E1$
HRG57R	$C_{13}R$
HRG60E	$C_{14}E1$
HRG60R	$C_{14}R$
HRG63E	$C_{15}E1$
HRG63R	$C_{15}R$
HRG66E	$C_{16}E1$
HRG66R	$C_{16}R$
HRG69E	$C_{17}E1$
HRG69R	$C_{17}R$
HRG72E	$C_{18}E1$
HRG72R	$C_{18}R$
HRG75E	C_nE1 (n>18)
HRG75R	C_nR (n>18)

TABLE XXIX. HYDROCARBON RADICALS - NOMENCLATURE INDEX

Dodecyl HR53E, HR53R

Ethene = ethylene
Ethenyl = vinyl
Ethenylene = vinylene
Ethenylidene = vinylidene
Ethinyl = ethynyl
Ethyl HR3E, HR3R
Ethylene HR6ER, HR6EE, HR6RR
Ethylidene HR7ER, HR7EE, HR7RR
Ethynyl HR5E, HR5R

Glyceryl = 1,2,3-propanetriyl

Hendecyl = undecyl
Hendecamethylene = undecamethylene
Heptadecamethylene HR70ER, HR70EE, HR70RR
Heptadecyl HR68E, HR68R
Heptamethylene HR38ER, HR38EE, HR38RR
Heptyl HR35E, HR35R
Hexadecamethylene HR67ER, HR67EE, HR67RR
Hexadecyl HR65E, HR65R
Hexamethylene HR34ER, HR34EE, HR34RR
Hexyl HR31E, HR31R

Isoallyl = propenyl
Isoamyl = isopentyl
Isobutyl HR21E, HR21R
Isoheptyl HR36E, HR36R
Isohexyl HR32E, HR32R
Isooctyl HR40E, HR40R
Isopropylidene HR16ER, HR16EE, HR16RR
Isopentyl HR26E, HR26R
Isopropyl HR11E, HR11R

Lauryl = dodecyl

Methene = methylene
Methylene HR2ER, HR2EE, HR2RR
Methyl HR1E, HR1R

Myristyl = tetradecyl

Neopentyl HR27E, HR27R
Nonamethylene HR46ER, HR46EE, HR46RR
Nonyl HR44E, HR44R

Octadecamethylene HR73ER, HR73EE, HR73RR
Octadecyl HR71E, HR71R
Octamethylene HR43ER, HR43EE, HR43RR
Octyl HR39E, HR39R
tert-Octyl = 1,1,3,3-tetramethylbutyl

Palmityl = hexadecyl
Pentadecamethylene HR64ER, HR64EE, HR64RR
Pentadecyl HR62E, HR62R
Pentamethylene HR30ER, HR30EE, HR30RR
Pentyl HR25E, HR25R
tert-Pentyl HR28E, HR28R
Polymethylene, C_{19} and larger HR76ER, HR76EE, HR76RR
1,2,3-Propanetriyl HR19ERR, HR19EER, HR19EEE, HR19RRR
Propenyl HR13E, HR13R
2-Propenylidene = allylidene
Propyl HR10E, HR10R
sec-Propyl = isopropyl
Propylene HR17ER1, HR17ER2, HR17EE, HR17RR
Propylidene HR15ER, HR15EE, HR15RR

Stearyl = octadecyl

Tetradecamethylene HR61ER, HR61EE, HR61RR
Tetradecyl HR59E, HR59R
1,1,3,3-Tetramethylbutyl HR41E, HR41R
Tetramethylene HR24ER, HR24EE, HR24RR
Tridecamethylene HR58ER, HR58EE, HR58RR
Tridecyl HR56E, HR56R
Trimethylene HR14ER, HR14EE, HR14RR

Undecamethylene HR52ER, HR52EE, HR52RR
Undecyl HR50E, HR50R

Vinyl HR4E, HR4R
Vinylene HR8ER, HR8EE, HR8RR
Vinylidene HR9ER, HR9EE, HR9RR

2.2.11 Miscellaneous Keys

2.2.11.1 Inorganic Compound Key Code IN

Assigned to all non-carbon compounds and to the following carbon-containing compounds:

metal carbonates
metal hydrogen carbonates (metal bicarbonates)
metal cyanides
metal isocyanides
metal carbonyls, i.e., Metal$(CO)_n$ compounds
carbides, except acetylides

2.2.11.2 General Metal Key Code MF M

Assigned to all compounds which contain any element other than the following: H, B, C, Si, N, P, As, Sb, O, S, Se, Te, F, Cl, Br, I. For further discussion, see Molecular Formula Keys, page 10.

2.2.11.3 General Metal Cation Key Code CN

Assigned to any positively charged metal ion, including $\overset{+}{N}H_4$, displayed in a structured compound. Note: Key is not assigned if the charged metal is bonded to another atom or group.

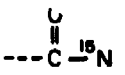
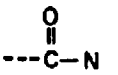
2.2.11.4 General Inorganic Anion Key Code AN

Assigned to any negatively charged atom or radical which functions as part of a structured compound but which, itself, is not structured. Note: The following carbon-containing anions are treated as inorganic: carbonate ($C\bar{O}_3$), bicarbonate ($HC\bar{O}_3$), cyanide ($C\bar{N}$), isocyanide ($N\bar{C}$).

2.2.11.5 Abnormal Mass (Isotope) Key Code MASS

Assigned to any compound containing a specified nuclide. Specified nuclides include deuterium (D), tritium (T), and any other atom whose symbol is accompanied by a numerical superscript at the left.

A structural fragment containing a specified nuclide is assigned the same key as the corresponding fragment without the specific nuclide. Example:

Fragment	Key
	

2.2.11.6 Compound Class Keys No general code

It is considered desirable to identify certain classes of compounds with specific keys. This would be reserved for classes which are difficultly structurable in toto or which contain no structural denominator common to all members of the class. Examples of such classes include: polyboranes, carbaboranes, polypeptides, alkaloids, glycosides, etc. Each class would receive a specific code which would be assigned automatically wherever possible and intellectually otherwise. No such keys are presently in the system.

3. ATOM-BY-ATOM SEARCH

CIDS retains the capability for computer probing the node-connector (atom-bond) table representation of a structure. One of the main features of the system, however, is to reduce to a minimum the need for this relatively expensive kind of searching. This reduction is effected through a maximally judicious use of the structural fragment component keys described in the previous sections of this report. It is expected that these keys will so restrict the population of compounds responsive to a query that a rapid printout of all retrieved structures is not only more economical but also more informative to the querist. Inasmuch as the purpose of this handbook is to display those features of the system which make for rapid automatic discrimination among structures, the details of conducting an atom-by-atom search are reserved for another publication.

4. CHEMICAL KEY ASSIGNMENT

All of the chemical search keys appropriate to a compound are automatically assigned to it by computer at the time it is registered in the CIDS file. While statistics have not yet been accumulated, it is evident from the disclosure (Sections 2 and 3) of the types of keys in the system that each compound will be tagged with numerous keys and that the number will increase as the complexity of the structure increases. Such wholesale type of key assignment is intentional in order that the compound will be responsive to the demands of queries involving various substructural features. It is emphasized that only a small family of these "total keys" will be needed in processing an individual query and that the composition of this small family will vary according to the specific demands of each query. Indeed, the fundamental principle involved in query formulation is to stipulate the minimum number of search keys required to define the query.

4.1 ILLUSTRATIVE EXAMPLES

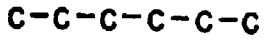
This section provides illustrations of the results of total key assignment to a wide variety of structural types of organic compounds drawn in the CIDS format and ordered roughly in the order of increasing complexity. Each illustration is presented on a separate page and consists of the following:

(1) the two-dimensional structural formula of the compound
(2) the total molecular formula and, where required, the dot-connected molecular formula
(3) the CIDS molecular formula keys assignable to the compound
(4) the specific A-C≈n key which serves to distinguish cyclic and acyclic compounds
(5) A listing of all CIDS structural fragment keys which would be assigned to the compound.

The listing of the keys in (5) above is in the same order that the key categories appear in Section 2.2 of this report. Especial attention is directed to the fact that in each case, the listing is confined to fragments actually present in the structure. Categories of keys not present in the structure are not included in the listing.

To facilitate comparison with the structure of the compound, the structural portrayal of each functional group and each hydrocarbon radical assigned to the compound are shown in parentheses.

EXAMPLE 1



C_6H_{14}

MF C 6
MF H 14
MF N 0
MF O 0

Key A-C=O

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

EXAMPLE 2

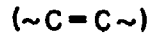
C_4H_8

MF C 4
MF H 8
MF N 0
MF C 0

Key A-C=0

Fragment Keys

EC1=1
EC2=0
EC3=0
EC4=0
NCN=0

FG120 

EXAMPLE 3

C_4H_6

MF C 4
MF H 6
MF N 0
MF O 0

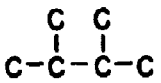
Key A-C=O

Fragment Keys

EC1=0
EC2=1
EC3=0
EC4=0
NCN=0

FG118 (---C≡C---)

EXAMPLE 4



C_6H_{14}

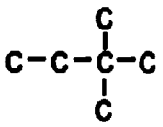
MF C 6
MF H 14
MF N 0
MF O 0

Key A-C=O

Fragment Keys

EC1=0
EC2=0
EC3=2
EC4=0
NCN=0

EXAMPLE 5



C_6H_{14}

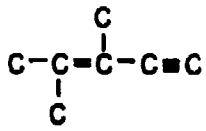
MF C 6
MF H 14
MF N 0
MF O 0

Key A-C=O

Fragment Keys

EC1=O
EC2=O
EC3=O
EC4=1
NCN=O

EXAMPLE 6



C_7H_{10}

MF C 7
MF H 10
MF N 0
MF O 0

Key A-C=O

Fragment Keys

EC1=1
EC2=1
EC3=2
EC4=0
NCN=0

FG120 (~C=C~)

FG118 (---C≡C---)

EXAMPLE 7

C_2F_2

MF C 2
MF F 2
MF N 0
MF O 0
MF F

Key A-C=0

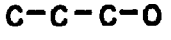
Fragment Keys

EC1=0
EC2=1
EC3=0
EC4=0
NCN=0

2 FG268 (-X)

2 FG121 (~C≡C-E|~)

EXAMPLE 8



C_3H_8O

MF C 3
MF H 8
MF O 1
MF N 0

Key A-C=O

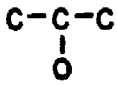
Fragment Keys

EC1=O
EC2=O
EC3=O
EC4=O
NCN=O

FG80 (---C-O)

HR10E (C-C-C-El~)

EXAMPLE 9



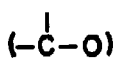
C_3H_8O

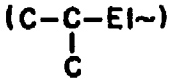
MF C 3
MF H 8
MF O 1
MF N 0

Key A-C=O

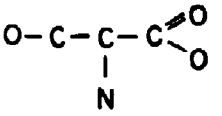
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

FG81 

HR11E 

EXAMPLE 10



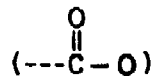
$C_3H_7NO_3$

MF C 3
MF H 7
MF N 1
MF O 3

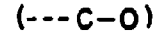
Key A-C=O

Fragment Keys

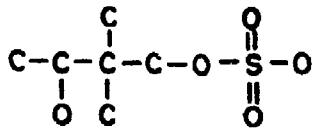
EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

FG94 

FG143 

FG80 

EXAMPLE 11



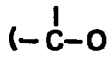
$C_6H_{14}O_5S$

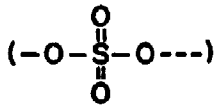
MF C 6
MF H 14
MF O 5
MF S 1
MF N 0
MF S

Key A-C=O

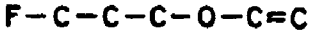
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=1
NCN=0

FG81 

FG232 

EXAMPLE 12



C_5H_9FO

MF C 5
MF H 9
MF F 1
MF O 1
MF N 0
MF F

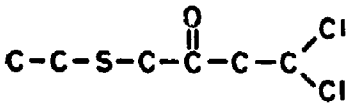
Key A-C=O

Fragment Keys

EC1=1
EC2=0
EC3=0
EC4=0
NCN=0

FG112	(---C-X)
FG178	(-O-)
FG120	(~C=C~)
HR4E	(C=C-EI~)
HR14EE	(~EI-C-C-C-EI~)

EXAMPLE 13



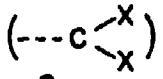
$C_6H_{10}Cl_2OS$

MF C 6
MF H 10
MF Cl 2
MF O 1
MF S 1
MF N 0
MF Cl
MF S

Key A-C=O

Fragment Keys

.Cl=O
EC2=O
EC3=O
EC4=O
NCN=O

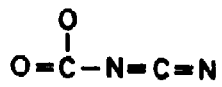
FG115 

FG86 

FG246 (–S–)

HR3E (C–C–El~)

EXAMPLE 1a



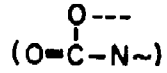
$C_2H_2N_2O$

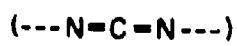
MF C 2
MF H 2
MF N 2
MF O 2

Key A-C=O

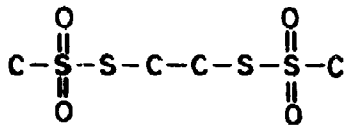
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

FG52 

FG62 

EXAMPLE 15



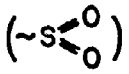
$C_4H_{10}O_4S_4$

MF C 4
MF H 10
MF O 4
MF S 4
MF N 0
MF S

Key A-C=0

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

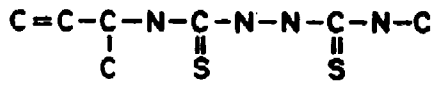
2 FG208 

2 FG251 (~S-S~)

2 HR1E (C-E!~)

HR6EE (~E!-C-C-E!~)

EXAMPLE 16



$C_7H_{14}N_4S_2$

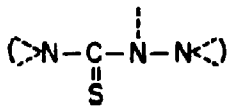
MF C 7
MF H 14
MF N 4
MF S 2
MF O 0
MF S

Key A-C=0

Fragments:

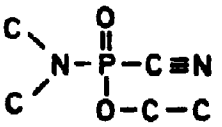
EC1 1
EC2=0
EC3=0
EC4=0
NCN=0

FG120 (~C=C~)

2 FG79 

HR1E (C-E I~)

EXAMPLE 17



$C_5H_{11}N_2O_2P$

MF C 5
MF H 11
MF N 2
MF O 2
MF P 1
MF P

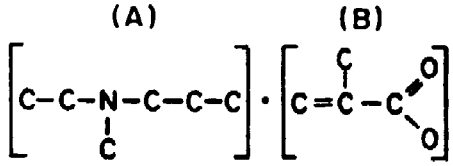
Key A-C=O

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

FG25 (~C≡N)
2 ND31 (~P~O~)
ND23 (~N~P)
2 HR1E (C-E|~)
HR3E (C-C-E|~)

EXAMPLE 18



$C_{10}H_{21}NO_2$

$C_6H_{15}N \cdot C_4H_6O_2$

MF C 10
MF H 21
MF N 1
MF O 2

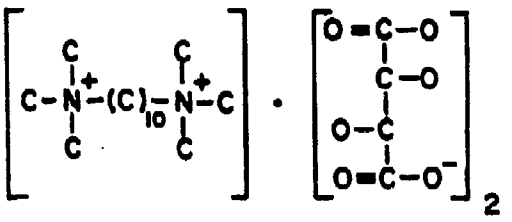
Key A-C=O

Fragment Keys

Structure (A)		Structure (B)	
EC1=0		EC1=1	
EC2=0		EC2=0	
EC3=0		EC3=1	
EC4=0		EC4=0	
NCN=0		NCN=0	
FG145	(-N-)	FG94	(---C(=O)-O)
		FG120	(~C=C~)
HR1E	(C-E|~)		
HR3E	(C-C-E|~)		
HR10E	(C-C-C-E|~)		

EXAMPLE 19

(A) (B)

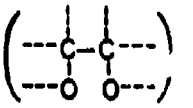
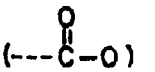


$C_{24}H_{48}N_2O_{12}$

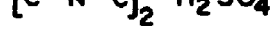
MF C 24
MF H 48
MF N 2
MF O 12

Key A-C=O

Fragment Keys

Structure (A)		Structure (B)	
EC1=0		EC1=0	
EC2=0		EC2=0	
EC3=0		EC3=0	
EC4=0		EC4=0	
NCN=0		NCN=0	
2 FG147	(~N+)	FG131	
		2 FG94	
HR49EE	(~E|-(C)$_{10}$-E|~)		
6 HR1E	(C-E|~)		

EXAMPLE 20



$C_4H_{16}N_2O_4S$

$2C_2H_7N \cdot H_2O_4S$

MF C 4
MF H 16
MF N 2
MF O 4
MF S 1
MF S

Key A-C=0

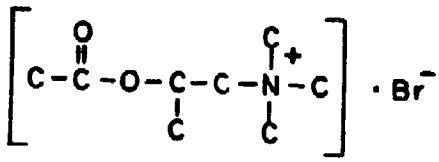
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

FG144 (-N-)

2 HR1E (C-E1~)

EXAMPLE 21



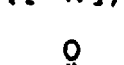
$C_8H_{18}BrNO_2$

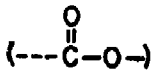
MF C 8
MF H 18
MF Br 1
MF N 1
MF O 2
MF Br

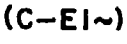
Key A-C=0

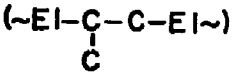
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=0

FG147 

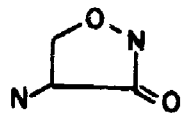
FG96 

3 HR1E 

HR17EE 

AN (Inorganic anion)

EXAMPLE 22



$C_3H_6N_2O_2$

MF C 3
MF H 6
MF N 2
MF O 2

Key A-C=1

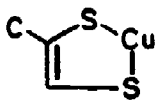
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=2
GCN1=1
GCN2=5
GCN3=C3 N1 O1
GCN4=C3 N1 O1
GCN5=0
GCN6=1,2
SCN11

FG143R (-N)

FG87 (C=O)

EXAMPLE 23



$C_3H_4CuS_2$

MF C 3
MF H 4
MF S 2
MF Cu
MF N 0
MF O 0
MF S

Key A-C=1

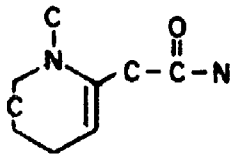
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=1
GCN1=1
GCN2=5
GCN3=C2 S2 UH1
GCN4=C2 S2 UH1
GCN5=1
GCN6=1,3,2

HR1R (C-R)

MF M (general metal molecular formula key)

EXAMPLE 24



$C_9H_{16}N_2O$

MF C 9
MF H 16
MF N 2
MF O 1

Key A-C=1

Fragment Keys

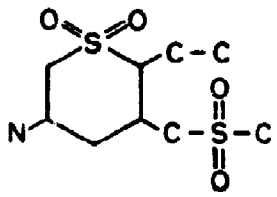
EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=2
GCN1=1
GCN2=7
GCN3=C6 N1
GCN4=C6 N1
GCN5=1

FG34 (---C(=O)-N)

HR1R (C-R)

HR1E (C-E|~)

EXAMPLE 25



$C_9H_{19}I$

MF C 9
MF H 19
MF N 1
MF O 4
MF S 2
MF S

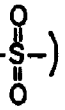
Key A-C=1

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=5
GCN1=1
GCN2=6
GCN3=C5 S1
GCN4=C5 S1
GCN5=0

FG143R (–N)

2 FG181 (([EI=O)

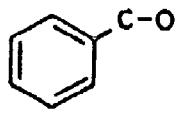
FG207 

HR1E (C–EI~)

HR2ER (R–C–EI~)

HR3R (C–C–R)

EXAMPLE 26



C_7H_8O

MF C 7
MF H 8
MF O 1
MF N 0

Key A-C=1

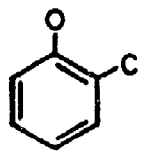
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=1
GCN1=1
GCN2=6
GCN3=C6
GCN4=C6
GCN5=3
SCN48

FG80R (---C-O)

HR2ER (R-C-E|~)

EXAMPLE 27



C_7H_8O

MF C 7
MF H 8
MF O 1
MF N 0

Key A-C=1

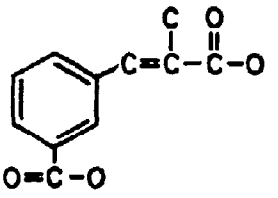
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=2
GCN1=1
GCN2=6
GCN3=C6
GCN4=C6
GCN5=3
SCN48

FG83 (C-O)

HR1R (C-R)

EXAMPLE 28



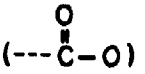
$C_{11}H_{10}O_4$

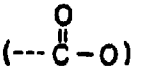
MF C 11
MF H 10
MF O 4
MF N 0

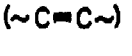
Key A-C=1

Fragment Keys

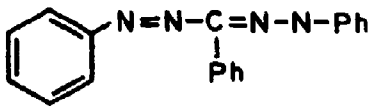
EC1=1
EC2=0
EC3=1
EC4=0
NCN=1
DACN=2
GCN1=1
GCN2=6
GCN3=C6
GCN4=C6
GCN5=3
SCN48

FG94 

FG94R 

FG120R 

EXAMPLE 29



$C_{19}H_{16}N_4$

MF C 19
MF H 16
MF N 4
MF O 0

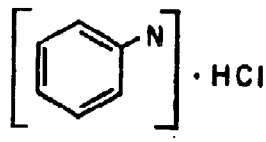
Key A-C=3

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=3
DACN=3
3 GCN1=1
3 GCN2=6
3 GCN3=C6
3 GCN4=C6
3 GCN5=3
3 SCN48

FG172R (–N=N–)
FG32 (~C=N~)
ND30 (~N~N~)

EXAMPLE 30



C_6H_8ClN

$C_6H_7N \cdot HCl$

MF C 6
MF H 8
MF Cl 1
MF N 1
MF O 0
MF Cl

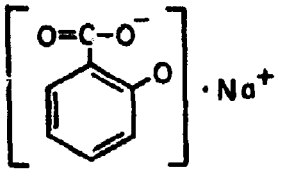
Key A-C=1

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=1
GCN1=1
GCN2=6
GCN3=C6
GCN4=C6
GCN5=3
SCN48

FG143R (-N)

EXAMPLE 31



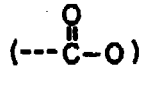
$C_6H_5NaO_3$

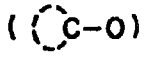
MF C 6
MF H 5
MF O 3
MF N 0
MF Na

Key A-C=1

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=2
GCN1=1
GCN2=6
GCN3=C6
GCN4=C6
GCN5=3
SCN48

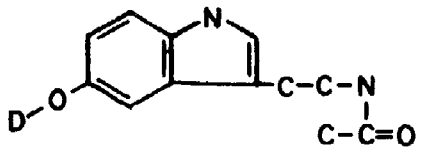
FG94R 

FG83 

MF M (general metal molecular formula key)

CN (general metal cation key)

EXAMPLE 32



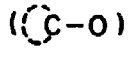
$C_{12}H_{13}DN_2O_2$

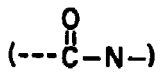
MF C 12
MF H 13
MF N 2
MF O 2
MF D

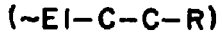
Key A-C=2

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=2
GCN1=2
GCN2=5,6
GCN3=C4 N1
GCN3=C6
GCN4=C8 N1
GCN5=4
SCN79

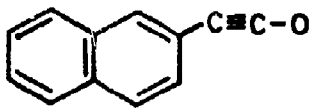
FG83 

FG35 

HR6ER 

MASS (Isotope)

EXAMPLE 33



$C_{12}H_8O$

MF C 12
MF H 8
MF O 1
MF N 0

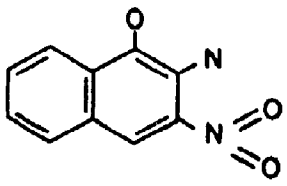
Key A-C=2

Fragment Keys

EC1=0
EC2=1
EC3=0
EC4=0
NCN=1
DACN=1
GCN1=2
GCN2=6,6
GCN3=C6
GCN3=C6
GCN4=C10
GCN5=5
SCN108

FG121R (~C≡C-E|~)
FG84 (~C-O)

EXAMPLE 34



$C_{10}H_8N_2O_3$

MF C 10
MF H 8
MF N 2
MF O 3

Key A-C=2

Fragment Keys

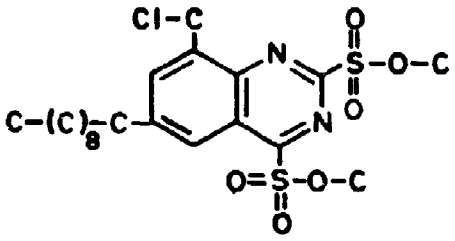
EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=3
GCN1=2
GCN2=6,6
GCN3=C6
GCN3=C6
GCN4=C10
GCN5=5
SCN108

FG83 (C–O)

FG143R (–N)

FG154R (–N=O)

EXAMPLE 35



$C_{21}H_{31}ClN_2O_6S_2$

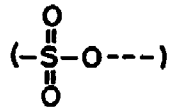
MF C 21
MF H 31
MF Cl 1
MF N 2
MF O 6
MF S 2
MF Cl
MF S

Key A-C=2

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=4
GCN1=2
GCN2=6,6
GCN3=C4 N2
GCN3=C6
GCN4=C8 N2
GCN5=5
SCN95

FG112R (---C-X)

2 FG223R 

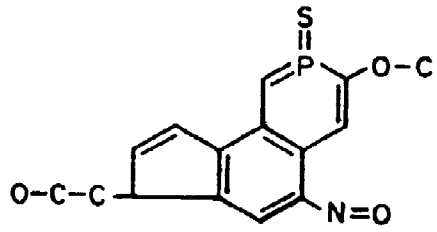
2 HR1E (C-E!~)

HR2ER (~E!-C-R)

HR47R $(C-(C)_8-C-R)$

HRG48R $(C_{10}-R)$

EXAMPLE 36



$C_{15}H_{14}NO_3PS$

MF C 15
MF H 14
MF N 1
MF O 3
MF P 1
MF S 1
MF P
MF S

Key A-C=3

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=4
GCN1=3
GCN2=5,6,6
GCN3=C5
GCN3=C5 P1
GCN3=C6
GCN4=C12 P1
GCN5=6

FG80 (---C-O)

FG249 (⬭ E1=S)

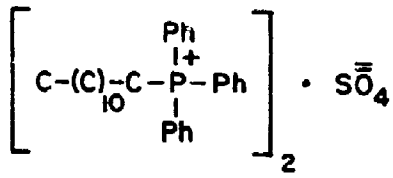
FG178R (-O-)

FG150R (-N=O)

HR1E (C-E1~)

HR6ER (R-C-C-E1~)

EXAMPLE 37



$C_{60}H_{80}O_4P_2S$

MF C 60
MF H 80
MF O 4
MF P 2
MF S 1
MF N 0
MF P
MF S

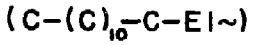
Key A-C=3

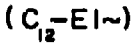
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=3
DACN=3

GCN1=	1	1	1
GCN2=	6	6	6
GCN3=	C6	C6	C6
GCN4=	C6	C6	C6
GCN5=	3	3	3
SCN	48	48	48

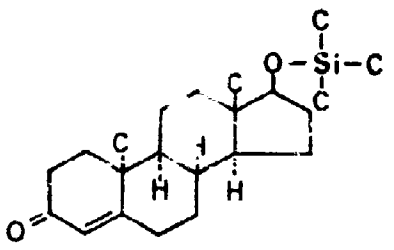
FG240 

HR53E 

HRG54E 

AN (Inorganic anion)

EXAMPLE 38



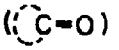
$C_{22}H_{36}O_2Si$

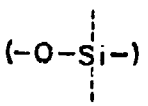
MF	C	22
MF	H	36
MF	O	2
MF	Si	1
MF	N	0
MF	Si	

Key A-C=4

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=4
GCN1=4
GCN2=5,6,6,6
GCN3=C5
GCN3=C6
GCN3=C6
GCN3=C6
GCN4=C17
GCN5=1
SCN130

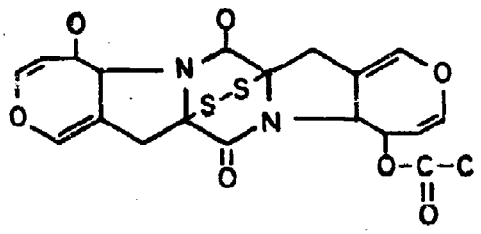
FG87 

FG193R 

3 HR1E (C-El~)

2 HR1R (C-R)

EXAMPLE 39



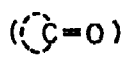
$C_{20}H_{18}N_2O_7S_2$

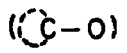
MF C 20
MF H 18
MF N 2
MF O 7
MF S 2
MF S

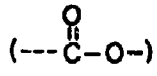
Key A-C=6

Fragment Keys

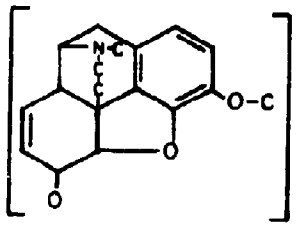
EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=4
GCN1=6
GCN2=5,5,6,6,7,7
GCN3=C4 N1
GCN3=C4 N1
GCN3=C3 N1 S2
GCN3=C3 N1 S2
GCN3=C6 O1
GCN3=C6 O1
GCN4=C18 N2 O2 S2
GCN5=4

2 FG87 

FG83 

FG96R 

EXAMPLE 40



$\cdot H_3PO_4 \cdot \frac{1}{2}H_2O$

$C_{18}H_{24}NO_7P \cdot \frac{1}{2}H_2O$

$C_{18}H_{21}NO_3 \cdot H_3PO_4 \cdot \frac{1}{2}H_2O$

MF C 18
MF H 24
MF N 1
MF O 7
MF P 1
MF P

Key A-C=5

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=1
DACN=3
GCN1=5
GCN2=5,6,6,6,6
GCN3=C4 O1
GCN3=C5 N1
GCN3=C6
GCN3=C6
GCN3=C6
GCN4=C16 N1 O1
GCN5=4

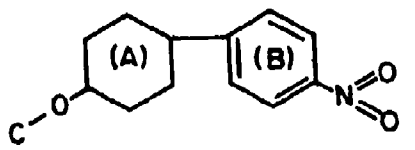
FG178R (-O-)

FG83 (C-O)

2 HR1E (C-E1~)

HR1R (C-R)

EXAMPLE 41



$C_{13}H_{17}NO_3$

MF C 13
MF H 17
MF N 1
MF O 3

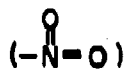
Key A-C=2

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=2
DACN=4

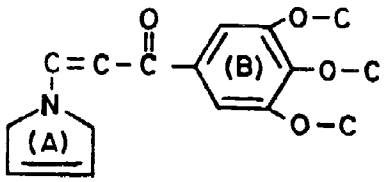
	Nucleus(A)	Nucleus(B)
GCN1=	1	1
GCN2=	6	6
GCN3=	C6	C6
GCN4=	C6	C6
GCN5=	0	3
SCN	49	48

FG178R (-O-)

FG154R 

HR1E (C-E|~)

EXAMPLE 42



$C_{16}H_{19}NO_4$

MF C 16
MF H 19
MF N 1
MF O 4

Key A-C=2

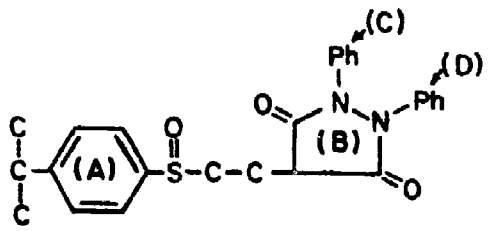
Fragment Keys

EC1=1
EC2=0
EC3=0
EC4=0
NCN=2
DACN=5

	Nucleus(A)	Nucleus(B)
GCN1=	1	1
GCN2=	5	6
GCN3=	C4 N1	C6
GCN4=	C4 N1	C6
GCN5=	1	3
SCN		48

FG86R	(-C-) with O
3 FG108R	(-O-)
FG120R	(~C=C~)
3 HR1F	(C-E I~)

EXAMPLE 43



$C_{26}H_{26}N_2O_3S$

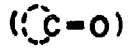
MF C 26
MF H 26
MF N 2
MF O 3
MF S 1
MF S

Key A-C=4

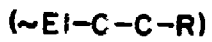
Fragment Keys

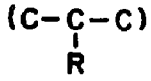
EC1=0
EC2=0
EC3=0
EC4=0
NCN=4
DACN=9

	Nucleus(A)	Nucleus(B)	Nucleus(C)	Nucleus(D)
GCN1=	1	1	1	1
GCN2=	6	5	6	6
GCN3=	C6	C3 N2	C6	C6
GCN4=	C6	C3 N2	C6	C6
GCN5=	3	0	3	3
GCN6=		1,2		
SCN	48	19	48	48

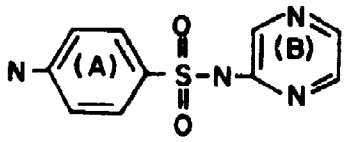
2 FG87 

FG187R 

HR6ER 

HR11R 

EXAMPLE 44



$C_{10}H_{10}N_4O_2S$

MF C 10
MF H 10
MF N 4
MF O 2
MF S 1
MF S

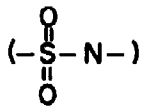
Key A-C=2

Fragment Keys

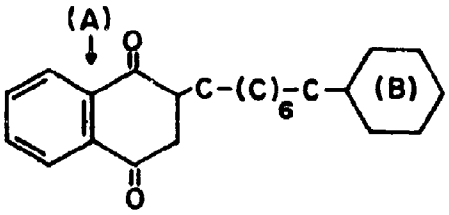
EC1=0
EC2=0
EC3=0
EC4=0
NCN=2
DACN=3

	Nucleus(A)	Nucleus(B)
GCN1=	1	1
GCN2=	6	6
GCN3=	C6	C4 N2
GCN4=	C6	C4 N2
GCN5=	3	3
GCN6=		1,4
SCN	48	41

FG143R (−N)

FG158R 

EXAMPLE 45



$C_{24}H_{34}O_2$

MF C 24
MF H 34
MF O 2
MF N 0

Key A-C=3

Fragment Keys

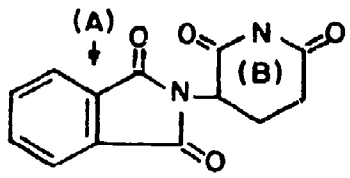
EC1=0
EC2=0
EC3=0
EC4=0
NCN=2
DACN=4

	Nucleus(A)	Nucleus(B)
GCN1=	2	1
GCN2=	6,6	6
GCN3=	C6	C6
GCN3=	C6	
GCN4=	C10	C6
GCN5=	3	0
SCN	109	49

2 FG87 (C=O)

HR43RR (R-(C)6-R)

EXAMPLE 46



$C_{13}H_{10}N_2O_4$

MF C 13
MF H 10
MF N 2
MF O 4

Key A-C=3

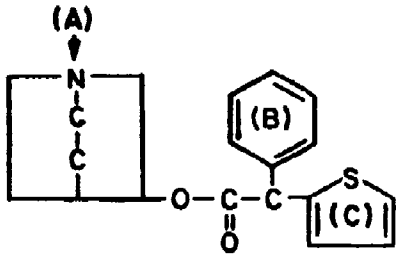
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=2
DACN=6

	Nucleus(A)	Nucleus(B)
GCN1=	2	1
GCN2=	5,6	6
GCN3=	C4 N1	C5 N1
GCN3=	C6	
GCN4=	C8 N1	C5 N1
GCN5=	3	0
SCN	82	45

4 FG87 (C=O)

EXAMPLE 47



$C_{19}H_{21}NO_2S$

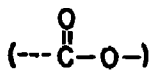
MF C 19
MF H 21
MF N 1
MF O 2
MF S 1
MF S

Key A-C=4

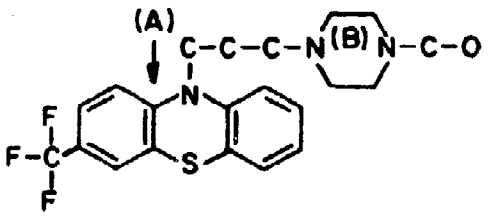
Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=3
DACN=3

	Nucleus(A)	Nucleus(B)	Nucleus(C)
GCN1=	2	1	1
GCN2=	6,6	6	5
GCN3=	C5 N1	C6	C4 S1
GCN3=	C5 N1		
GCN4=	C7 N1	C6	C4 S1
GCN5=	0	3	2
SCN	98	48	29

FG96R 

EXAMPLE 48



$C_{21}H_{24}F_3N_3OS$

MF C 21
MF H 24
MF F 3
MF N 3
MF O 1
MF S 1
MF F
MF S

Key A-C=4

Fragment Keys

EC1=0
EC2=0
EC3=0
EC4=0
NCN=2
DACN=4

	Nucleus(A)	Nucleus(B)
GCN1=	3	1
GCN2=	6,6,6	6
GCN3=	C4 N1 S1	C4 N2
GCN3=	C6	
GCN3=	C6	
GCN4=	C12 N1 S1	C4 N2
GCN5=	6	0
GCN6=		1,4
SCN	116	42

FG84R (~C-O)

FG117R (---C(X)(X)-X)

HR2EE (~E!-C-E!~)

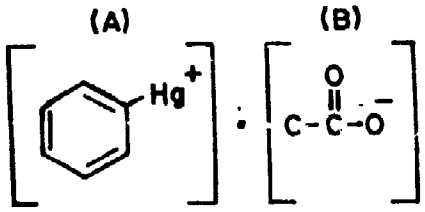
HR2ER (~E!-C-R)

HR14EE (~E!-(C)$_3$-E!~)

HR14ER (~E!-(C)$_3$-R)

HR14RR (R-(C)$_3$-R)

EXAMPLE 49



$C_8H_8HgO_2$

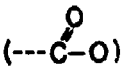
MF C 8
MF H 8
MF O 2
MF Hg
MF N 0

Key A-C=1

Fragment Keys

Structure(A)	Structure(B)
EC1=0	EC1=0
EC2=0	EC2=0
EC3=0	EC3=0
EC4=0	EC4=0
NCN=1	NCN=0
DACN=1	
GCN1=1	
GCN2=6	
GCN3=C6	
GCN4=C6	
GCN5=3	
SCN48	

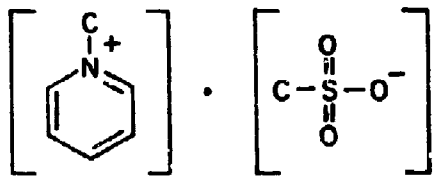
FG139R (-Hg~)

FG94 

MF M (general metal molecular formula key)

EXAMPLE 50

(A) (B)

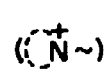
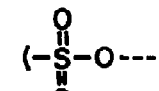


$C_7H_{11}NO_3S$

MF C 7
MF H 11
MF N 1
MF O 3
MF S 1
MF S

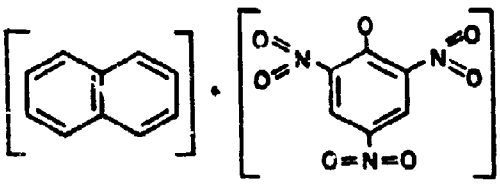
Key A-C=1

Fragment Keys

Structure(A)		Structure(B)	
EC1=0		EC1=0	
EC2=0		EC2=0	
EC3=0		EC3=0	
EC4=0		EC4=0	
NCN=1		NCN=0	
DACN=1			
GCN1=1			
GCN2=6			
GCN3=C5 N1			
GCN4=C5 N1			
GCN5=3			
SCN44			
FG146		FG223	
HR1R	(C–R)	HR1E	(C–E|~)
HR1E	(C–E|~)		

EXAMPLE 51

(A) (B)



$C_{16}H_{11}N_3O_7$

$C_{10}H_8 \cdot C_6H_3N_3O_7$

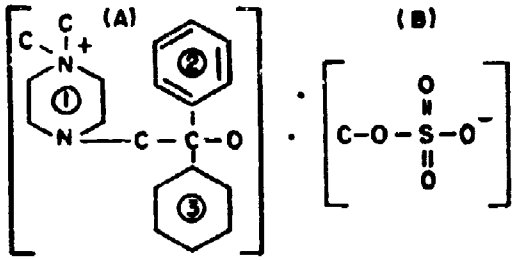
MF C 16
MF H 11
MF N 3
MF O 7

Key A-C=3

Fragment Keys

Structure(A)	Structure(B)
EC1=0	EC1=0
EC2=0	EC2=0
EC3=0	EC3=0
EC4=0	EC4=0
NCN=1	NCN=1
DACN=0	DACN=4
GCN1=2	GCN1=1
GCN2=6,6	GCN2=6
GCN3=C6	GCN=C6
GCN3=C6	
GCN4=C10	GCN4=C6
GCN5=5	GCN5=3
SCN108	SCN48
	FG83 (C-O)
	3 FG154R (-N(=O)=O)

EXAMPLE 52

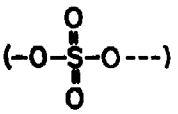
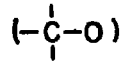


$C_{21}H_{36}N_2O_5S$

MF C 21
MF H 36
MF N 2
MF O 5
MF S 1
MF S

Key A-C=3

Fragment Keys

Structure(A)				Structure(B)
EC1=0				EC1=0
EC2=0				EC2=0
EC3=0				EC3=0
EC4=0				EC4=0
NCN=3				NCN=0
DACN=5				
	Nucleus(1)	Nucleus(2)	Nucleus(3)	
GCN1=	1	1	1	
GCN2=	6	6	6	
GCN3=	C4 N2	C6	C6	
GCN4=	C4 N2	C6	C6	
GCN5=	0	3	0	
GCN6=	1,4			
SCN	42	48	49	
FG146				FG232 
FG82R				
2 HR1E	(C-E!~)			HR1E (C-E!~)
2 HR1R	(C-R)			

LITERATURE CITED

1. C. T. Van Meter, D. Lefkovitz, and R. V. Powers, An Experimental Chemical Information and Data System, CIDS No. 4 Status Report, University of Pennsylvania, Philadelphia, Pa., January 1967

2. A. M. Patterson, L. T. Capell, and D. F. Walker, The Ring Index, Second Edition, American Chemical Society, Washington, D. C., November 1959, and Supplements

UNCLASSIFIED
Security Classification

DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) UNIVERSITY OF PENNSYLVANIA Philadelphia, Pennsylvania 19104	2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED 2b. GROUP NA

3. REPORT TITLE

HANDBOOK OF CIDS CHEMICAL SEARCH COMPONENTS

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

Status Report, CIDS No. 6 - January-December 1968

5. AUTHOR(S) (Last name, first name, initial)

Van Meter, Clarence T., Goldschmidt, Eric N., and Milne, Margaret

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
December 1968	208	2

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)
DA-18-035-AMC-288(A) b. PROJECT NO. c. Task: 2P062101A72702 d.	CIDS NO. 6/STATUS REPORT 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)

10. AVAILABILITY/LIMITATION NOTICES This document is subject to special export controls and each transmittal to a foreign national or a foreign government may be made only with prior approval of the Commanding Officer, Edgewood Arsenal, ATTN: SMUEA-TSTI-T, Edgewood Arsenal, Maryland 21010

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
Army chemical and information data systems	Edgewood Arsenal Technical Support Directorate, Edgewood Arsenal, Maryland 21010 (Stanley Goldberg, Proj. O., Ext 6126)

13. ABSTRACT This handbook is intended for use as a desk-top tool in the specification of molecular and structural characteristics of chemicals which are used as keys (screens) in queries addressed to a model operational CIDS. It subdivides the several hundred characteristics into conventional categories and identifies all of the individual characteristics within each category. Each category of keys is defined and the individual keys are CIDS-encoded and, where appropriate, structured. Numerous tables are provided arranged in such a way as to facilitate locating a particular key, and nomenclature indexes are available, where appropriate, for users who wish to employ a name approach. Illustrations of the total assignment of the keys to a variety of chemical compounds are presented.

14. KEY WORDS

CIDS chemical handbook
CIDS chemical search components
Molecular formula keys
Molecular formula statements
Structural fragment keys
Cyclic nuclei keys
Specific functional group keys
Nonspecific functional group keys
Hydrocarbon radical keys
Miscellaneous CIDS chemical keys
Isotopes
Atom-by-atom search
Chemical key assignment
Chemical nomenclature indexes

DD FORM 1 JAN 64 1473

UNCLASSIFIED
Security Classification